

Information and Computation: Classical and Quantum Aspects

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Quantum theory has found a new field of applications in the realm of information and computation during the recent years. This paper reviews how quantum physics allows information coding in classically unexpected and subtle nonlocal ways, as well as information processing with an efficiency largely surpassing that of the present and foreseeable classical computers. Some outstanding aspects of classical and quantum information theory will be addressed here. Quantum teleportation, dense coding, and quantum cryptography are discussed as a few samples of the impact of quanta in the transmission of information. Quantum logic gates and quantum algorithms are also discussed as instances of the improvement in information processing by a quantum computer. We provide finally some examples of current experimental realizations for quantum computers and future prospects.

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I. INTRODUCTION

The twentieth century we have just left behind opened with the discovery of quanta by Planck (1900) and followed with the formulation of the quantum theory during the first decades. As the century went by, we have witnessed a continuous and growing increase in the number of applications of quantum mechanics, which began with atomic physics and then the number kept growing (nuclear and particle physics, optics, condensed matter, . . .) and became countless. As the century was closing we have come across an unexpected new field of applications that have given quantum physics a refreshing twist, keeping the pace even with the newest trends of discoveries, such as the field of new technologies of information and computation. In a sense and having in mind the times we live, those of the information era and the new technologies, it seems inevitable that physics gets affected by the presence of computers all over around, which are more and more powerful and have revolutionized many areas of science. What is more surprising is the fact that quantum physics may influence the field of information and computation in a new and profound way, getting at the very root of their foundations. For instance, fundamental

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aspects of quantum mechanics such as those entering the EPR (Einstein, Podolsky and Rosen, 1935) states have found unexpected applications in information transmission and cryptography.

But, why has this happened? It all begun by realizing that information has physical nature (Landauer, 1991; 1996; 1961). It is printed on a physical support (the rocky wall of a cave, a clay tablet, a parchment, a sheet of paper, a magneto-optic disk, etc.), it cannot be transmitted faster than light in vacuum, and it abides by the natural laws. The statement that information is physical does not simply mean that a computer is a physical object, but in addition that information itself is a physical entity. In turn, this implies that the laws of information are restricted or governed by the laws of physics. In particular, those of quantum physics. In fact these ones, through their linearity, entanglement of states, nonlocality and indetermination principle make possible new and powerful transmission tools and information treatments, as well as a really prodigious efficiency of computation.

A typical computation is implemented through an algorithm in a computer. This algorithm is now regarded as a set of physical operations and the registers of the quantum computer are considered to be states of a quantum system. Moreover, the familiar operation of initializing the data for a program to run is replaced by the preparation of an initial quantum state, and the usual tasks of writing programs and running them correspond, in the new formulation, to finding appropriate Hamiltonians for their time evolution operators to lead to the desired output. This output is retrieved by a quantum measurement of the register, and this fact has deep implications on the way quantum information must be handled.

We shall see that information and computation blend well with quantum mechanics. Their combination brings unexpected results on the way information can be transmitted and processed, extending the capabilities known so far in the field of classical information to unsuspected limits, sometimes entering the realm of science-fiction, sometimes surpassing it.

The advance has been remarkable mainly in the field of cryptography, where it has provided systems absolutely secure for the quantum distribution of keys. Quantum computation is also one of the hot research fields in current physics; the same applies to the challenge posed by the experimental realization of a computer complex enough to implement the new algorithms that exploit the fantastic possibilities of the massive parallelism characterizing those quantum computers, and that would amount to a dramatic improvement for solving hard or classically untractable problems.

We first review the essentials of quantum information theory and then discuss several of their consequences and applications, some of them specifically quantum such as quantum teleportation, dense coding; some of them with a classical echo such as quantum cryptography. Next we review the fundamentals of quantum computation de-

scribing the notion of a quantum Turing machine and its practical implementation with quantum circuits. We describe the notion of elementary quantum gates for universal computation and how this extends the classical counterpart. We also provide a discussion of the basic quantum algorithms and finally we give a general overview of some of the possible physical realizations of quantum computers.

Both in the information and computation parts we make special emphasis in presenting first an introduction to the classical aspects of these disciplines in order to better clarify what quantum theory adds to them in the new formulations of these theories. Actually, this is also what we do in physics.

II. CLASSICAL INFORMATION

Information is discretized: it comes in irreducible packages. The elementary unit of classical information is the *bit* (or *cbit*, for classic bit), a classical system with only two states 0 and 1 (False and True, No and Yes, . . .). Any text can be coded into a string of bits: for instance, it is enough to assign to each symbol its ASCII code number in binary form, appended with a parity check bit. Example: **quanta** can be coded as

11100010 11101011 11000011 11011101 11101000 11000011

Each bit can be stored physically; in classical computers, each bit is registered as a charge state of a capacitor (0 = discharged, 1 = charged). They are distinguishable macroscopic states, and robust enough or stable. They are not spoiled when they are read in (if carefully done) and they can be cloned or replicated without any problem.

Information is not only stored; it is usually transmitted (communication), and sometimes processed (computation).

A. The Theorems of Shannon

The classical theory of information is due to Shannon (1948,1949), who in two seminal works definitively laid down its principles in 1948. With his celebrated *noiseless coding theorem* he showed how much *compressible* a message can be, or equivalently, how much redundancy it has. Likewise with his *coding theorem in a noisy channel* he also found what is the minimum redundancy that must be present into a message in order to be *comprehensible* when reaching the receiver, despite of the noise.

Let $A := \{a_1, \dots, a_{|A|}\}$ be a finite alphabet, endowed with a probability distribution $p_A : a_i \mapsto p_A(a_i)$, with $\sum_{1 \leq i \leq |A|} p_A(a_i) = 1$. Sometimes we shall write this as $A := \{a_i, p_A(a_i)\}_{i=1}^{|A|}$. Let us consider messages or character strings $x_1 x_2 \dots x_n \in A^n$, originating from a memoryless source, i.e., a symbol a appears in a given

place with probability $p_A(a)$, independently of the symbols entering the remaining sites in the chain.¹ The first Shannon's theorem asserts that, if $n \gg 1$, the information supplied by a generic message of n characters (and thus $(n \log_2 |A|)$ -bits long) essentially coincides with that transmitted by another shorter message, of bit length $nH(A)$, where H is the so called Shannon's entropy

$$H(A) = - \sum_{1 \leq i \leq |A|} p_A(a_i) \log_2 p_A(a_i) \in [0, \log_2 |A|]. \quad (1)$$

In other words, each character is compressible up to $H(A)$ bits on the average; moreover, this result is optimal (Welsh, 1995; Roman 1992; Schumacher, 1995; Preskill, 1998).

The basic idea underlying the proof is simple: it amounts to take notice only of the *typical* messages. Let us assume for clarity a binary alphabet ($A = \{0, 1\}$). Let $p, 1-p$ be the probabilities of 0,1, respectively. In a long message of n bits ($n \gg 1$), there will be approximately np 0s. Let us call typical messages those with a number of 0s of the order of np . Asymptotically ($n \rightarrow \infty$), there are $2^{nH(A)}$ many of them, among a total of 2^n messages. The probability $P : (x_1, \dots, x_n) \mapsto p(x_1) \dots p(x_n)$ of the messages ($n \gg 1$)-bits long tends to get concentrated on this reduced ensemble consisting of the typical strings, which explains Shannon's result. The atypical messages are ignorable in probability. It suffices to transmit through the communication channel (assumed perfect, noiseless) the binary number of length $nH(A)$ assigned to each typical message upon common agreement between the sender and the recipient, so that the emitted message can be identified on reception.² The optimality of Shannon's first theorem is easily arguable: all $2^{nH(A)}$ typical sequences are asymptotically equiprobable and thus they cannot be represented faithfully with less than $nH(A)$ bits.

If the transmission channel is noisy (the common case), the information fidelity gets lost, since some bits may get corrupted along the way. To fight the noise of a given channel one resorts to redundancy, by cleverly coding each symbol with more bits than strictly necessary so that the erroneous bits might be easily detected and restored. A price is paid however, since the transmission of essential information gets clearly slower. Shannon's wonderful second theorem quantifies this issue.

¹The natural languages are not like these (for instance, in the usual Spanish there exists no digram like QÑ). Nevertheless, they can be considered, to a good approximation, as limit of ergodic Markovian languages to which the Shannon theorem can be extended (Welsh, 1995).

²There exist very practical methods for classical coding with an efficiency close to the optimal value, such as the Huffman code (Roman, 1992), with multiple applications (facsimile, digital TV, etc.). The essence of this code is to assign shorter binary strings to the most frequent symbols.

Let X be the alphabet of the transmitter station (of a memoryless source), and Y be the one of the receiver station. Let $(p_{Y|X}(y_j|x_i))$ be the stochastic matrix for that channel, with entries given by the probabilities that the input symbol $x_i \in X$ appears as $y_j \in Y$ on output. The marginal probability distribution for Y is given by $p_Y(y_j) = \sum_i (p_{Y,X}(y_j, x_i) := \sum_i p_{Y|X}(y_j|x_i) p_X(x_i))$. The channel ability to transmit information is measured by its *capacity* $C := \sup_{p_X} I(X : Y) = \max_{p_X} I(X : Y)$, where $I(X : Y) = I(Y : X)$ is the *mutual information*

$$I(X : Y) := \sum_j \sum_i p_{Y,X}(y_j, x_i) \log_2 \frac{p_{Y,X}(y_j, x_i)}{p_Y(y_j) p_X(x_i)} \quad (2)$$

or the information about X (Y) conveyed by Y (X). The convexity of the log makes $I(X : Y) \geq 0$ (knowing Y can never lower the information about X).

The capacity C may be viewed as the number of output bits per input symbol which are correctly transmitted. Its computation is usually very difficult.

Many channels are binary symmetric: each transmitted bit has the same probability p of being reversed, i.e., of being erroneous upon arrival. These are the channels considered here. For them we have $C = 1 - H_2(p) := C(p)$, with $H_2(p) := -p \log_2 p - (1-p) \log_2 (1-p)$. Note that $C(\frac{1}{2}) = 0$, being such a channel totally useless for transmission since it transforms any input binary word into a random output sequence. Thus we will assume that $p < \frac{1}{2}$.

In the transmission of a word $w \in \{0, 1\}^n$, an error $e \in \{0, 1\}^n$ may be produced such that the received word is $w' = w + e$ (addition mod 2). A subset of words $C_n \subset \{0, 1\}^n$ encoding (i.e. in bijective correspondence with) a collection of messages is said to be an *error-correcting classical code* (ECCC) for $e \in \mathcal{E}_n \subset \{0, 1\}^n$ if $(w + \mathcal{E}_n) \cap (w' + \mathcal{E}_n) = \emptyset$ for any $w \neq w' \in C_n$. That is, no matter the distortion produced by the errors on a codeword $w \in C_n$, there is no overlapping between the different sets $w + \mathcal{E}_n$, and the decoding is possible without ambiguities. If upon previous agreement, it is known which specific message corresponds to each codeword, it will be enough to send this one instead of the message; the latter will be capable of being recovered at the other side of the channel after "cleaning-up" the received word from the possible errors which can affect it. In this way the transmitted codeword can be identified and its decoding done afterwards. In the practical use of a code C_n , mistakes can occur in the restoration of the messages, caused by errors outside \mathcal{E}_n , that is, out of the security framework of the code. But as long as the frequency of failures remains very low, the risk will be bearable. It is apparent that for this to happen it will be convenient to put very distant apart (in the Hamming sense, that is, in the number of bits in which they differ) the different words of the code, for the possibility that the errors will cause collisions between two distinct words of code will diminish in this fashion.

One defines the *rate* of the code C_n as $R := \log_2 |C_n|/n$. It measures the number of informative bits per transmit-

ted bit. It is easy to argue that in order for the code to be reliable, its rate must not overcome the capacity of the channel: $R \leq C$. In fact, when transmitting a codeword w with length n , there will be produced a number of np reversed bits on average, and hence an error e which will be likely one of the $2^{nH_2(p)}$ typical sequences. For the decoding to be reliable, there should be no overlapping between the error spheres with centers at the codewords, and thus $2^{nH_2(p)}|\mathcal{C}_n| \leq 2^n$, thereby $R \leq C$. This result suggests that the capacity C is an upper bound to all faithful transmission rates.

The second Shannon's theorem closes this issue in the asymptotic limit. Suppose given a binary symmetric channel, a transmission rate R not exceeding the capacity of the channel ($0 < R < C$), an $\epsilon > 0$ arbitrarily small and any sequence $\{N_n\}_1^\infty$ of integers such that $1 \leq N_n \leq 2^{nR}$. Then, the theorem asserts that there exist codes $\{\mathcal{C}_n \subset \mathbb{Z}_2^n\}_1^\infty$ with N_n elements (codewords), appropriate decision schemes for decoding, and an integer $n(\epsilon)$, such that the *fidelity* $F(\mathcal{C}_n)$ or probability that a given decoded message coincides with the original is $\geq 1 - \epsilon$ (that is, the maximum probability of error in the identification of the codeword on reception is $\leq \epsilon$) for all $n \geq n(\epsilon)$ (Roman, 1992; Welsh, 1995). Moreover, it is possible to make the error probabilities to tend to 0, exponentially in n .

The theorem is optimal: the capacity C should not be exceeded if the transmission is to be faithful. As a matter of fact, it is known that for each sequence of codes $\{\mathcal{C}_n\}_1^\infty$ with $|\mathcal{C}_n| = \lceil 2^{nR} \rceil$, whose rate exceeds the capacity of the channel ($R > C$), the average error probability tends asymptotically to 1.

The proof of this Shannon's theorem relies on codes chosen at random and decoding schemes based on the maximum likelihood principle; unfortunately, it is not constructive, but existential, leaving open the practical problem of finding out codes which cleverly combine a good efficiency in correcting errors, a simple decoding and a high rate.

B. Classical Error Correction

Errors in the storage and processing of the information are unavoidable. A classical way of correcting them is resorting to *redundancy* (repetition codes): each bit is substituted by a string of $n \geq 3$ bits equal to it,

$$0 \mapsto \underbrace{00\dots 00}_n, \quad 1 \mapsto \underbrace{11\dots 11}_n, \quad (3)$$

and, if by any chance, an error occurs in such a way that one of the bits in one of those strings gets reversed (for instance $00000 \mapsto 01000$), to correct the error it is enough to invoke the majority vote. Let p be probability for any bit to get spoiled. In general, several bits of the n -tuple may be reversed. When $p < \frac{1}{2}$, the probability for the majority rule to fail can be made as smaller as desired,

taking n sufficiently large. It is apparent that if the n -tuples of bits are systematically and frequently examined, so that it is very unlikely that errors occur at two or more bits, then the application of this simple method will clean-up the n -tuples from errors and their error-free state will be restored. However, the price to pay might be too high since with codes of length n sufficiently large so as to insure a small error during the detection, the transmission rate can turn up prohibitively small (in our case it is $1/n$ source bits per channel bit).

So far, we have been describing correction codes $\mathcal{C} \subset \{0,1\}^n$ for errors in $\mathcal{E} \subset \{0,1\}^n$. More generally, we can consider q -ary alphabets (whose symbols we shall assume to be the elements of the finite field \mathbb{F}_q with $q = p^f$ elements, p being a prime). Given two words $x, y \in \{0,1,\dots,q-1\}^n$, let $d_H(x,y)$ be its Hamming distance (number of locations in which x, y differ). Let $d := d_H(\mathcal{C}) := \inf_{x \neq y \in \mathcal{C}} d_H(x,y)$ be the minimum distance of the code. Then, the code \mathcal{C} allows the correction of errors that affect to a maximum number $t := \lfloor \frac{1}{2}(d-1) \rfloor$ of positions:³ it is enough to replace each received word by the closest codeword in the Hamming metric.⁴ Therefore, the most convenient codes are those with a high d , but this is at the expense of decreasing $|\mathcal{C}|$. If M is the number of codewords, we shall call it a $(n, M, d)_q$ code. Its rate is defined as $R := n^{-1} \log_q M$.

When \mathcal{C} is a linear subspace of \mathbb{F}_q^n , the code is called *linear*. Therefore the linear codes are of the form $(n, q^k, d)_q$, where k is the dimension of the linear subspace \mathcal{C} ; for them d coincides with the minimal Hamming length of a non-vanishing codeword, and the searching of the codeword nearest to each received word is greatly simplified. It is customary to represent them as $[n, k, d]_q$, or simply as $[n, k]_q$ when d is irrelevant. Their rate is k/n . Given a code \mathcal{C} of type $[n, k]_q$, the matrix G , $k \times n$, with rows given by the components of the vectors in a basis of \mathcal{C} is called a *generator matrix* for \mathcal{C} . Defining now in \mathbb{F}_q^n a scalar product in the canonical way, we can introduce the *dual* code \mathcal{C}^\perp of \mathcal{C} . A generator matrix H for \mathcal{C}^\perp is known as a *parity-check matrix* for \mathcal{C} ; notice that $\mathcal{C} = \{u \in \mathbb{F}_q^n : Hu = 0\}$, what justifies in part the name given to H , for it allows us to easily “check” whether a vector in \mathbb{F}_q^n belongs or not to the subspace \mathcal{C} .

The coding applies bijectively and linearly \mathbb{F}_q^k onto a code $\mathcal{C} \subset \mathbb{F}_q^n$ of type $(n, q^k, d)_q$, and it is implemented as follows. Let $\{e_1, \dots, e_k\} \subset \mathbb{F}_q^n$ be a basis of \mathcal{C} . Given a source word $w^t = (w_1, \dots, w_k) \in \mathbb{F}_q^k$, it gets assigned a codeword $c(w) := \sum_i w_i e_i$. In terms of the generator matrix, $w^t \mapsto w^t G$. Let us call $\pi : w \mapsto c(w)$ this injection. During the transmission, $c(w)$ could get corrupted,

³Notation: $\lfloor x \rfloor$ ($\lceil x \rceil$) is the largest (smallest) integer $\leq x$ ($\geq x$).

⁴For instance, for the repetition code $\mathcal{C} = \{0\dots 0, 1\dots 1, \dots, (q-1)\dots(q-1)\}$, with q codewords of length n , we have $d = n$, and thus it exactly corrects $\lfloor (n-1)/2 \rfloor$ errors.

becoming $u := c(w) + e$, where $e \in \mathcal{E}$ is a possible error vector. It is evident that $e \in u + \mathcal{C}$. In order to decode it, the criterion of minimal Hamming distance is applied, replacing u by $\pi^{-1}(u - u_0)$, where u_0 is an element of the coset $u + \mathcal{C}$ which minimizes the distance to the origin (such u_0 is known as a *leader* of $u + \mathcal{C}$). The linearity of the code allows us to economize in this last step. We make a look-up table containing for each coset $v + \mathcal{C} \in \mathbb{F}_q^n/\mathcal{C}$ its *syndrome* Hv (which uniquely characterizes the coset) and a leader v_0 . Upon receiving u as a message, the syndrome Hu is computed and its corresponding leader u_0 is searched in the table; next, decoding proceeds as stated before (Macwilliams and Sloane, 1977; Roman, 1992; Welsh, 1995). The original message is faithfully retrieved iff the error coincides with one of the leaders in the table.

Some of the most relevant linear codes are (Macwilliams and Sloane, 1977; Roman, 1992; Welsh, 1995):

1. The repetition code $\mathcal{C} = \{0 \dots 0, 1 \dots 1, \dots, (q-1) \dots (q-1)\}$ is of type $[n, 1, n]_q$, and although for it the minimum distance is optimal, its rate is dreadful.

2. The Hamming codes $H_q(r)$ are arguably the most famous of them all. They are codes of the type $[n = 1 + q + \dots + q^{r-1}, k = n - r, d = 3]_q$, and they are *perfect*, in the sense that the set of Hamming spheres with radius $\lfloor (d-1)/2 \rfloor$ and center at each codeword fill \mathbb{F}_q^n . These codes have rates $R = 1 - r/n$ which tend to 1 as $n \rightarrow \infty$, but they only correct one error.

For instance, $H_2(3)$ is of type $[7, 4, 3]_2$ and rate $4/7$. A parity-check matrix for this code is

$$H = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix}. \quad (4)$$

Its decoding is particularly simple. Let u be the word received instead of the codeword w , and assume that u has only one corrupted bit. The syndrome $s(u) := Hu$ coincides in this case with the binary expression of the position occupied by the erroneous bit. Negating this single bit will thus suffice to clean the word to get the correct codeword. For example, if $u = 0110001$, then $s(u) = 110$, so that the incorrect bit is the sixth one, and hence $w = 0110011$.

3. The Golay codes G_{24} and G_{23} are binary, of type $[24, 12, 8]_2$ and $[23, 12, 8]_2$, respectively. They are probably the most important codes.

The code G_{24} is *self-dual*, i.e. $\mathcal{C} = \mathcal{C}^\perp$, what simplifies decoding. Its rate is $R = 1/2$, and allows the correction of up to 3 errors; it was used by NASA in 1972-82 for the transmission of color images of Jupiter and Saturn from the Voyagers.

The code G_{23} is *perfect*, and it gives rise to G_{24} when augmented with a parity bit.

The Golay codes G_{12} and G_{11} are ternary, of type $[12, 6, 6]_3$ and $[11, 6, 5]_3$, respectively. As before, G_{12} is self-dual, while G_{11} is perfect and originates G_{12} when appended with a parity bit.

The codes G_{24} and G_{12} have very peculiar combinatorial properties; their groups of automorphisms are M_{24} and $2.M_{12}$, where M_{24} y M_{12} are the famous sporadic groups of Mathieu. This latter group is the subgroup of S_{12} generated by two special permutations of 12 cards labeled from 0 to 11: $0, 1, 2, \dots, 11 \mapsto 11, 10, 9, \dots, 0$ and $0, 1, 2, \dots, 11 \mapsto 0, 2, 4, 6, 8, 10, 11, 9, 7, 5, 3, 1$. It is also the group of motions of the form $\tau_i \tau_j^{-1}$ on a “Rubick” icosahedron, where τ_i indicates a rotation of angle $2\pi/5$ degrees around the i -th axis of the icosahedron (Conway and Sloane, 1999). As a matter of fact, it was the discovery of the Golay codes what drove further the study of the sporadic groups which resulted into the complete classification of the finite simple groups, with the discovery by Griess in 1983 of the “monster” or “friendly giant” group, finite and simple, an enormous subgroup of $SO(47 \times 59 \times 71)$ with about 10^{54} elements.

4. The Reed-Muller binary codes $RM(r, m)$, with $0 \leq r \leq m$, are of type $[n = 2^m, k = \sum_{k \leq r} \binom{m}{k}, d = 2^{m-r}]_2$. Their rates, for fixed r , tend to 0 when increasing m . They rank among the oldest codes known. The code $RM(1, 5)$, of type $(32, 64, 16)_2$, is able to correct up to 7 errors with a rate of $R = 3/16$. It was used in 1969-72 to transmit from the Mariners the white-and-black photos of Mars.

5. The Reed-Solomon codes generalize the Hamming codes. They have been heavily employed by NASA in the transmission of information during the Galileo, Ulysses and Magellan missions to the deep outer space, and currently they are used all over, from CD-ROMs to the hard-disks of computers.

6. The algebraic-geometric Goppa codes $G_q(D, G)$ are in turn interesting generalizations of the Reed-Solomon codes. They have allowed to obtain families of codes *asymptotically good*, that is, families containing infinite sequences $\{[n_i, k_i, d_i]_q\}$ of codes, with $n_i \rightarrow \infty$, such that the sequences $\{k_i/n_i, d_i/n_i\}$ of rates and minimum relative distances are bounded from below by certain positive numbers (Macwilliams and Sloane, 1977; Roman, 1992; Stichtenoth, 1993; Blake et al., 1998).

1. Some asymptotic bounds for linear codes

To obtain good encodings it is advisable to use long codes which permit not only sending many different messages but also present a large minimum distance which allows for correcting sufficiently many errors. Given a code $\mathcal{C} = [n, k, d]_q$, let $R(\mathcal{C}) := k/n$ be its rate and $\delta(\mathcal{C}) := d/n$ its minimum relative distance. A theorem of Manin asserts that the set of limit points of $\{(\delta(\mathcal{C}), R(\mathcal{C})) \in [0, 1]^2 : \mathcal{C} \text{ is a code on } \mathbb{F}_q\}$ is of the form $\{(\delta, R) \in [0, 1]^2 : \delta \in [0, 1], 0 \leq R \leq \alpha_q(\delta)\}$, where $\alpha_q(\delta)$ is a continuous function of $\delta \in [0, 1]$, decreasing in $[0, 1 - q^{-1}]$, and such that $\alpha_q(0) = 1$, $\alpha_q(\delta) = 0$ if $1 - q^{-1} \leq \delta \leq 1$ (256).

Let H_q be the q -ary entropy function $H_q(x \in [0, 1 - q^{-1}]) := x \log_q(q-1) - x \log_q x - (1-x) \log_q(1-x)$. The

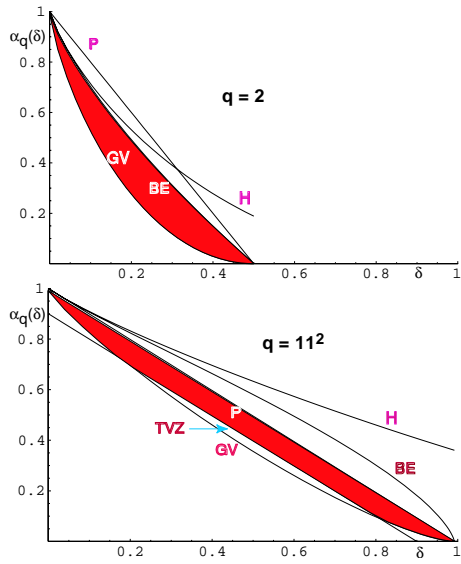


FIG. 1: Asymptotic bounds. The dark zone is limited by the lower and upper bounds mentioned in the text.

following bounds for the function $\alpha_q(\delta)$ in the relevant interval $\delta \in [0, 1 - q^{-1}]$ are known (39, 230, 256):

- Plotkin's upper bound:

$$\alpha_q(\delta) \leq 1 - (1 - q^{-1})^{-1}\delta \quad (5)$$

- Hamming's or sphere-packing upper bound:

$$\alpha_q(\delta) \leq 1 - H_q(\delta/2) \quad (6)$$

- Bassaligo-Elias' upper bound:

$$\alpha_q(\delta) \leq 1 - H_q(\theta - \sqrt{\theta(\theta - \delta)}), \text{ con } \theta := (1 - q^{-1}) \quad (7)$$

- Gilbert-Varshamov' lower bound:

$$\alpha_q(\delta) \geq 1 - H_q(\delta) \quad (8)$$

This last one is very important, since it ensures the existence of codes as long as desired with minimum relative distance δ and rate R both asymptotically positive.

- Tsfasman-Vlăduț-Zink' lower bound: if q is a square, then on $[0, 1 - (\sqrt{q} - 1)^{-1}]$ one has

$$\alpha_q(\delta) \geq \left(1 - \frac{1}{\sqrt{q} - 1}\right) - \delta \quad (9)$$

which is stronger than Gilbert-Varshamov' bound in some places from $q = 7^2$ on.

For an illustration see Fig. 1.

The quantum information theory, being an extension of the classical theory, is essentially a product of the past decade (Bouwmeester, Ekert and Zeilinger, 2000; Nielsen and Chuang, 2001).

In quantum information, the analogue of the classical bit is called *qubit* or *quantum bit* (Schumacher, 1995). It is a two-dimensional quantum system (for instance, a spin $\frac{1}{2}$, a photon polarization, an atomic system with two relevant states, etc.), with Hilbert space isomorphic to \mathbb{C}^2 . Besides the two basis states $|0\rangle, |1\rangle$, the system can have infinitely many other (pure) states given by a coherent linear superposition $\alpha|0\rangle + \beta|1\rangle$. The Hilbert space of n qubits is the tensor product $\mathbb{C}^2 \otimes \dots \otimes \mathbb{C}^2 = \mathbb{C}^{2^n}$, and its natural basis vectors are $|0\rangle \otimes \dots \otimes |0\rangle =: |0\dots 0\rangle$, $|0\rangle \otimes \dots \otimes |1\rangle =: |0\dots 1\rangle, \dots, |1\rangle \otimes \dots \otimes |1\rangle =: |1\dots 1\rangle$. For this basis, also known as the computational basis, we shall assume the lexicographic ordering. When appropriate, we shall briefly write $|x\rangle$ to denote $|x_{n-1}\dots x_0\rangle$, with $x := x_0 + 2x_1 + \dots + 2^{n-1}x_{n-1}$. Thus, $|5\rangle = |0\dots 0101\rangle$.

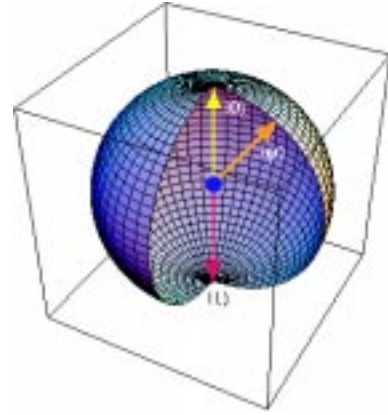


FIG. 2: Parameterization of the states of one qubit: the Bloch sphere.

There exists the possibility of extending the two-level qubits to *qudits* or d -dimensional systems ($d \geq 2$) (Rungta et al., 2000). This leads to an extension of the binary quantum logic. Using d computational levels we can reduce the number n_2 of qubits needed for a computation by a factor of $\lfloor \log_2 d \rfloor$, since the Hilbert space of n_d qudits contains the space of n_2 qubits provided that $d^{n_d} \geq 2^{n_2}$.

Given an arbitrary state vector $|\Psi\rangle = c_0|0\rangle + c_1|1\rangle$ of a qubit, the complex coefficients $c_0, c_1 \in \mathbb{C}$ amount to 4 real parameters. However, if we parameterize them as $c_i = r_i e^{i\phi_i}, i = 0, 1$ and factor out a global irrelevant phase, we find $|\Psi\rangle = r_0|0\rangle + r_1 e^{i(\phi_1 - \phi_0)}|1\rangle$. Imposing $|\Psi\rangle$ to be of unit norm, we can write it as

$$|\psi\rangle = (\cos \frac{1}{2}\theta)|0\rangle + e^{i\phi}(\sin \frac{1}{2}\theta)|1\rangle \quad (10)$$

where r_0, r_1 are now parameterized by the angles $\theta, \phi := \phi_1 - \phi_0$.

These two angles represent a point in a S^2 sphere, called the Bloch sphere, as shown in Fig. 2. Thus, the (projective) Hilbert space of pure states of a single qubit can be parameterized by the points on this sphere. As a byproduct, this construction provides a nice representation of the “classical” bits as particular points on the sphere. The classical bit 0 (better the qubit state $|0\rangle$) marks the north pole and the 1 sits on the south pole. Any other point on the sphere amounts to a non-trivial linear superposition of the basis states. The angle θ is related to the proportion of $|1\rangle$ to $|0\rangle$ in the composition of that state, while the angle ϕ is their relative quantum phase.

It leaps to the eye from Fig. 2 that the information contained in a qubit is infinite as compared to the information in a classical bit. In other words, at a given time, a bit can take on only one of the two values, either 0 or 1, while a qubit can be in any of the infinitely many possible quantum states in (10). As we shall see later in detail, this fact is basic to what is known as “quantum parallelism”, a source of the unprecedented capabilities exhibited by a quantum computer.

A *quantum logic gate*⁵ acting on a collection or *quantum register* of k qubits is just any unitary operator in the associated Hilbert space \mathbb{C}^{2^k} (Deutsch, 89). For instance, besides the identity, we have for 1 qubit the 1-ary gates X (or U_{NOT}), Y , Z , given by the Pauli matrices σ_a (in the natural basis $\{|0\rangle, |1\rangle\}$):

$$U_{\text{NOT}} := X := \sigma_x, \quad Y := -i\sigma_y, \quad Z := \sigma_z. \quad (11)$$

The particular linear combination $U_H := 2^{-1/2}(X + Z)$ is the important *Hadamard gate*.

The unary gates are easy to implement (for instance, on polarized photons, with $\frac{1}{2}\lambda$, $\frac{1}{4}\lambda$ plates).

On 2 qubits, the most important gate is *controlled NOT* (U_{CNOT}), or *exclusive OR* (U_{XOR}), defined by $U_{\text{CNOT}}, U_{\text{XOR}} : |x\rangle|y\rangle \mapsto |x\rangle|x \oplus y\rangle$, where x, y are either 0, 1, and \oplus means addition mod 2. This gate can be represented by the matrix

$$\begin{aligned} U_{\text{CNOT}} &:= U_{\text{XOR}} := |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes U_{\text{NOT}} \\ &= \frac{1}{2}(1 + \sigma_z) \otimes 1 + \frac{1}{2}(1 - \sigma_z) \otimes \sigma_x. \end{aligned} \quad (12)$$

The physical implementation of this gate is central to the applications of quantum information and will be addressed later in Sec. XI.

The quantum partner of the Shannon entropy is the Von Neumann entropy

$$S(\rho) := -\text{Tr}(\rho \log_2 \rho), \quad (13)$$

where ρ is the density operator describing a normal quantum state. Given a convex decomposition $\rho = \sum_{i \in I} p_i |\phi_i\rangle\langle \phi_i|$ in pure states, it can be shown that $S(\rho) \leq H(I) := -\sum_i p_i \log_2 p_i$, equality holding if and only if the state vectors ϕ_i are pairwise orthogonal. The Von Neumann entropy has the well-known properties of concavity, strong subadditivity and triangularity (Thirring, 1983; Galindo and Pascual, 1990a; Galindo and Pascual, 1989):

$$\begin{aligned} \lambda_1 S(\rho_1) + \lambda_2 S(\rho_2) &\leq S(\lambda_1 \rho_1 + \lambda_2 \rho_2), \\ S(\rho_{ABC}) + S(\rho_B) &\leq S(\rho_{AB}) + S(\rho_{BC}), \\ |S(\rho_A) - S(\rho_B)| &\leq S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B), \end{aligned} \quad (14)$$

with $\lambda_{1,2} \geq 0$, $\lambda_1 + \lambda_2 = 1$. The subscripts A, B, C denote subsystems.

The first two relations also hold in the classical theory of information. But the third property (whose second part is just the property of simple subadditivity) is peculiar. While in Shannon’s theory the entropy of a composite system can never lower the entropy of any of its parts, quantumly this is not the case. The EPR states of the form $2^{-1/2}(|aa'\rangle + |bb'\rangle)$,⁶ where a, b and a', b' are given orthonormal pairs, provide us with an explicit counterexample.

2. No-cloning theorem

A basic difference between classical and quantum information is that while classical information can be copied perfectly, quantum cannot. This is relevant to quantum communication protocols for should a quantum copier exist, then safe eavesdropping of quantum channels would be possible. In particular, we cannot create a duplicate of a quantum bit in an unknown state without uncontrollably perturbing the original. This follows from the no-cloning theorem of Wootters and Zurek (1982). The statement is the following: let $\mathcal{H} := \mathcal{H}_{\text{orig}} \otimes \mathcal{H}_{\text{copy}}$ be the joint Hilbert space of the original and of the copy, and let U_{QCM} be the linear (unitary) operator in \mathcal{H} representing the action of an alleged *quantum copier machine*:

$$U_{\text{QCM}} : |\Psi\rangle_{\text{orig}} |\phi_0\rangle \mapsto |\Psi\rangle_{\text{orig}} |\Psi\rangle_{\text{copy}}, \quad \forall |\Psi\rangle \in \mathcal{H}_{\text{orig}}, \quad (15)$$

where $|\phi_0\rangle$ is the “blank” state of the copy.

We claim that such a machine cannot exist. This is a remarkably simple application of the linearity of quantum mechanics. For a contradiction, suppose it does exist. Assume for simplicity that the object to copy is just a single qubit, and let $|\Psi\rangle_{\text{orig}} = \alpha_0|0\rangle + \alpha_1|1\rangle$. Then, linearity implies

$$U_{\text{QCM}} |\Psi\rangle |\phi_0\rangle = \alpha_0 |0\rangle |0\rangle + \alpha_1 |1\rangle |1\rangle \quad (16)$$

⁵A more extended study of quantum logic gates and their classical counterparts is presented in Sec. IX.B and Sec. VIII.D.

⁶Actually, they are EPR states à la Bohm, that is, EPRB states (Bohm, 1951).

whereas the definition of a quantum copier yields

$$\begin{aligned} U_{\text{QCM}}|\Psi\rangle|\phi_0\rangle &= |\Psi\rangle|\Psi\rangle \\ &= \alpha_0^2|0\rangle|0\rangle + \alpha_0\alpha_1|0\rangle|1\rangle + \alpha_1\alpha_0|1\rangle|0\rangle + \alpha_1^2|1\rangle|1\rangle \end{aligned} \quad (17)$$

The results (16), (17) are in general incompatible, what proves the assertion.

A more general proof of the no-cloning theorem takes into account the environment and makes use of the unitarity of U_{QCM} : now $\mathcal{H} := \mathcal{H}_{\text{orig}} \otimes \mathcal{H}_{\text{copy}} \otimes \mathcal{H}_{\text{env}}$, and

$$U_{\text{QCM}}|\Psi\rangle_{\text{orig}}|\phi_0\rangle|E_0\rangle = |\Psi\rangle_{\text{orig}}|\Psi\rangle_{\text{copy}}|E_\Psi\rangle, \forall |\Psi\rangle \in \mathcal{H}_{\text{orig}}, \quad (18)$$

where $|E_0\rangle$ is the “rest” state of the “remaning world” (environment) before copying, and $|E_\Psi\rangle$ its state after copying. Let us consider two actions of the QCM,

$$\begin{aligned} U_{\text{QCM}}|\Psi_1\rangle|\phi_0\rangle|E_0\rangle &= |\Psi_1\rangle|\Psi_1\rangle|E_{\Psi_1}\rangle \\ U_{\text{QCM}}|\Psi_2\rangle|\phi_0\rangle|E_0\rangle &= |\Psi_2\rangle|\Psi_2\rangle|E_{\Psi_2}\rangle. \end{aligned} \quad (19)$$

Taking the scalar product of these two actions and using unitarity yields $\langle\Psi_1|\Psi_2\rangle = \langle\Psi_1|\Psi_2\rangle^2 \langle E_{\Psi_1}|E_{\Psi_2}\rangle$. Therefore, since all these probability amplitudes have modulus ≤ 1 , then either $\langle\Psi_1|\Psi_2\rangle = 0$ or 1, and hence copying two different and non-orthogonal states Ψ_1, Ψ_2 is impossible.

However, a known quantum state can be copied at will. Moreover, dropping the requirement that copies be perfect, approximate quantum copying machines may exist (Buzek and Hillery, 1996). Should it be possible to make close to perfect copies then quantum cryptographic schemes might still be at risk. Quantum copying can also become essential in storage and retrieval of information in quantum computers.

A. Entanglement and Information

A quantum pure state $|\Psi\rangle$ in a Hilbert space $\mathcal{H} = \bigotimes_{i=1}^n \mathcal{H}_i$ of n qubits is said to be *separable* (with respect to the factor spaces $\{\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_n\}$) when it can be factorized as follows:

$$|\Psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle, |\psi_i\rangle \in \mathcal{H}_i. \quad (20)$$

Otherwise the state $|\Psi\rangle$ is called *entangled*. Famous examples of entangled states are the EPR pairs (Einstein, Podolsky and Rosen, 1935) or Bell states like

$$\begin{aligned} |\Psi^\pm\rangle &:= \frac{1}{\sqrt{2}}[|01\rangle \pm |10\rangle] \\ |\Phi^\pm\rangle &:= \frac{1}{\sqrt{2}}[|00\rangle \pm |11\rangle] \end{aligned} \quad (21)$$

which physically may be represented by a spin- $\frac{1}{2}$ singlet and triplet or by entangled polarized (vertical and horizontal) photons (Kwiat et al., 1995), and the GHZ state (Greenberger, Horne and Zeilinger, 1989)

$$|\text{GHZ}\rangle := \frac{1}{\sqrt{2}}[|000\rangle + |111\rangle], \quad (22)$$

which has been observed experimentally in polarization entanglement of three spatially separated photons (Bouwmeester et al., 1999).

The concept of entanglement is the distinctive and responsible feature that allows quantum information to overcome some of the limitations posed by classical information, as exemplified by the new phenomena of teleportation, dense coding, etc., to be explained in the following sections. Although it is simple to state mathematically, entanglement leads however to profound experimental consequences like non-local correlations: when two distant apart parties A (Alice) and B (Bob) share say an EPR pair,⁷ the measurement by A of her state univocally determines the state on the B side. Apparently, this implies instant information transmission, in sharp contrast with Einstein’s relativity. However, to reconcile both facts we must notice that the only way the B side has to know about his state (without measuring it) is by receiving a classical communication from the A side, which does propagate no faster than the speed of light.

For these basic reasons, entanglement is considered as a resource in quantum information (Bennett, 1998), something that we must have available if we want to take advantage of the new communication possibilities exhibited by quantum protocols.

When the system has two parts, namely $\mathcal{H} := \mathcal{H}_A \otimes \mathcal{H}_B$, it is called *bipartite*. In general, a *multipartite* system is of the form $\mathcal{H} := \bigotimes_{i=1}^n \mathcal{H}_i$. We may think of entanglement as a manifestation of the superposition principle when applied to bipartite or multipartite systems. Thus, genuine multiparticle or many-body states exhibit entanglement properties, which in the theory of strongly correlated systems are known as quantum correlations (Fulde, 1993).⁸ We may state that entanglement and quantum correlations are closely linked.

Being a non-local concept, entanglement must be independent of local manipulations performed on each of the A and B parties. These operations are represented by unitary operators $U_A \otimes U_B$, in a factorized form, acting on the states of $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, or they may be local measurements on either side. Moreover, classical communication is also permitted by the two parties. Entanglement cannot be created by these local operations. However, factorized states can be obtained by local operations, like measurements. Altogether, these type of local operations plus classical communications are known as LOCC transformations. The set LOCC is not a group, but a semigroup for the inverse of a given transformation

⁷It is usual in information theory to introduce a set of characters named as Alice (the sender), Bob (the recipient), and Eve (the eavesdropper).

⁸These type of correlations are responsible for novel quantum phase transitions (Sachdev, 1999) where the transition is driven by quantum fluctuations instead of standard thermal fluctuations.

is not guaranteed to exist, due to possible irreversible measurements by each party.

The characterization of entanglement for general quantum states (pure or mixed, bipartite or multipartite) is very difficult, in part due to the type of transformations allowed in the set LOCC. For entangled pure states of 2 qubits or general bipartite systems A and B with dimensions d_A, d_B respectively, entanglement is well understood in terms of their Schmidt (1906) decomposition: given an arbitrary state

$$|\Psi\rangle_{AB} := \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} C_{ij} |a_i\rangle_A |b_j\rangle_B \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \quad (23)$$

with $\{|a_i\rangle_A\}_1^{d_A}, \{|b_i\rangle_B\}_1^{d_B}$ orthonormal bases of $\mathcal{H}_A, \mathcal{H}_B$, then it admits a biorthonormal decomposition of the form

$$|\Psi\rangle_{AB} = \sum_{k=1}^r \sqrt{w_k} |u_k\rangle_A |v_k\rangle_B, \quad w_k > 0, \quad \sum_{k=1}^r w_k = 1, \quad (24)$$

where $\{|u_k\rangle_A\}_1^r$ and $\{|v_k\rangle_B\}_1^r$ are sets of orthonormal vectors for subsystems A and B, and $r \leq d := \min\{d_A, d_B\}$ is the so called *Schmidt rank* of $|\Psi\rangle_{AB}$ (Schmidt, 1906; Hughston, Jozsa and Wootters, 1993; Ekert and Knight, 1995).⁹ The coefficients w_k are called *Schmidt weights*.

The Schmidt decomposition is essentially unique in the following sense: the weights (multiplicities included) are unique (up to order), and hence the rank; given a non-degenerate weight w_k , the state vectors $|u_k\rangle_A, |v_k\rangle_B$, are unique up to reciprocal phase factors; when the weight w_k is degenerate, the corresponding states in Alice's side are unique up to an arbitrary unitary transformation U_A to be compensated by a simultaneous unitary transformation $U_B = U_A^*$ on the associated vectors in Bob's side.

From the Schmidt decomposition it immediately follows that a bipartite pure state $|\Psi\rangle_{AB}$ is entangled if and only if its Schmidt rank $r > 1$.

From the point of view of the subsystem A, the description of its quantum properties is realized by means of the *reduced density matrix* ρ_A (and likewise for subsystem B with ρ_B):

$$\begin{aligned} \rho_A &:= \text{Tr}_B |\Psi\rangle_{AB} \langle \Psi| \\ \rho_B &:= \text{Tr}_A |\Psi\rangle_{AB} \langle \Psi| \end{aligned} \quad (25)$$

where Tr_B denotes the *partial trace* over the B subsystem (similarly for Tr_A and subsystem B). The Schmidt

decomposition (24) implies that

$$\begin{aligned} \rho_A &= \sum_{k=1}^r w_k |u_k\rangle_A \langle u_k| \\ \rho_B &= \sum_{k=1}^r w_k |v_k\rangle_B \langle v_k| \end{aligned} \quad (26)$$

Another important implication of (24) is that as $r \leq d$, when a qubit state $d_A = 2$ is entangled to a qudit state $d_B \geq 2$ then the Schmidt decomposition has at most two terms, no matter how large d_B is.

Interestingly enough, the Schmidt decomposition has appeared independently again in the field of strongly correlated systems through the density matrix renormalization group method DMRG (White, 1992; 1993).¹⁰

Once we know whether a given bipartite pure state is entangled or not, next question is to get entanglement ordered: given two states $|\Psi_1\rangle_{AB}, |\Psi_2\rangle_{AB}$, which one is more entangled? No sufficiently general answer is known to this question. A tentative simple choice would be to measure entanglement through the partial Von Neumann entropies (Bennett et al., 1996a):

$$E(|\Psi_{AB}\rangle) := S(\rho_A) = S(\rho_B) \quad (27)$$

Such entropies do not increase under LOCC, but having $E(|\Phi_{AB}\rangle) < E(|\Psi_{AB}\rangle)$ does not guarantee that an LOCC action may bring $|\Psi_{AB}\rangle$ to $|\Phi_{AB}\rangle$.

The *theory of majorization* provides us with a criterion to ascertain when any two entangled states can be LOCC connected (Nielsen, 1999). Given two vectors $x = (x_1, x_2, \dots, x_d), y = (y_1, y_2, \dots, y_d)$ in \mathbb{R}^d , decreasingly ordered $x_1 \geq x_2 \geq \dots x_d, y_1 \geq y_2 \geq \dots y_d$, we say that x is *majorized* by y , denoted $x \prec y$, (equivalently, y *majorizes* x) if the following series of relations hold true:

$$\begin{aligned} x_1 &\leq y_1 \\ x_1 + x_2 &\leq y_1 + y_2 \\ &\vdots \\ x_1 + x_2 \dots x_{d-1} &\leq y_1 + y_2 \dots y_{d-1} \\ x_1 + x_2 \dots x_d &= y_1 + y_2 \dots y_d \end{aligned} \quad (28)$$

The majorization relation is a partial order in \mathbb{R}^d : 1/ $x \prec x, \forall x$; 2/ $x \prec y$ and $y \prec x$ iff $x = y$; 3/ if $x \prec y$ and $y \prec z$ then $x \prec z$. When the components of the vector x are positive $x_k \geq 0$ and normalized $\sum_k x_k = 1$, they may be thought of as probability distributions as is Sec. II. The central result is the following: a bipartite state $|\Psi\rangle_{AB}$

⁹The Schmidt decomposition is equivalent to the *Singular Value Decomposition* (SVD) of the $d_A \times d_B$ matrix $C := (C_{ij})$ in linear algebra (Press et al., 1992). Let $d_A \leq d_B$. Then $C = UDV^t$, where U is an orthogonal $d_A \times d_A$ matrix ($U^t U = 1_{d_A}$), V is a $d_A \times d_B$ matrix representing a Euclidean isometry from \mathbb{C}^{d_A} to \mathbb{C}^{d_B} (i.e. $VV^t = 1_{d_A}$), and D is the $d_A \times d_A$ diagonal matrix $\text{diag}(\sqrt{w_1}, \dots, \sqrt{w_r}, 0, \dots, 0)$. Using the SVD $C_{ij} = \sum_{k=1}^{d_A} U_{ik} \sqrt{w_k} V_{jk}$ in (23) we immediately arrive at the Schmidt decomposition (24).

¹⁰The Schmidt weights govern the truncation process inherent to the DMRG method: the highest weights are retained while the smallest (beyond a certain desired value) are eliminated. This truncation makes the exponentially large problem much more amenable.

can be transformed via LOCC operations into another state $|\Phi\rangle_{AB}$ iff $w(|\Psi\rangle)$ is majorized by $w(|\Phi\rangle)$,

$$|\Psi\rangle_{AB} \longrightarrow |\Phi\rangle_{AB} \iff w(|\Psi\rangle) \prec w(|\Phi\rangle) \quad (29)$$

where $w(|\Psi\rangle)$ is the ordered vector of eigenvalues or weights (multiplicities included) of the reduced density matrix ρ_A (25),(26) associated with $|\Psi\rangle_{AB}$ (similarly for $w(|\Phi\rangle)$).

For example, let us consider the parties A and B sharing this couple of qutrit states in the basis $\{|0\rangle, |1\rangle, |2\rangle\}$:

$$\begin{aligned} |\Psi\rangle_{AB} &= \frac{2}{3}|00\rangle + \frac{2}{3}|11\rangle + \frac{1}{3}|22\rangle \\ |\Phi\rangle_{AB} &= \sqrt{\frac{2}{3}}|00\rangle + \sqrt{\frac{1}{6}}|11\rangle + \sqrt{\frac{1}{6}}|22\rangle \end{aligned} \quad (30)$$

Both states are entangled, but $|\Psi\rangle_{AB}$ cannot be transformed into $|\Phi\rangle_{AB}$ or viceversa: they possess different types of entanglement. They are said to be *incomparable* or *incommensurate* (Nielsen, 1999; Vidal, 1999).

However, for general multipartite systems the issue of how to relate the LOCC action with entanglement in a given pure state is an open question (Lewenstein et al., 2000).

A definition of entanglement for finite dimensional systems with mixed states characterized by a density matrix ρ goes as follows (Werner, 1989): ρ is called separable when it can be written as a convex combination of product states

$$\rho = \sum_{k=1}^r \lambda_k \otimes_{j=1}^n \rho_k^{(j)}, \quad \lambda_k \geq 0, \quad \sum_k \lambda_k = 1. \quad (31)$$

When ρ is not separable, one calls it an entangled mixed state. The situation about quantifying and qualifying entanglement is even worse for mixed quantum states (Horodecki et al., 1996a; Peres, 1996; Dür, Cirac and Tarrach, 1999; Giedke et al., 2001). There are partial characterizations of entanglement like the Peres criterion (1996): a necessary condition for separability of ρ is that the matrices $\rho^{t,j}$, $j = 1, \dots, r$, obtained by *partial transposition*¹¹ of ρ with respect to an arbitrary orthonormal basis of the factor space \mathcal{H}_j of the j -component, is non-negative ($\rho^{t,j} \geq 0$). The converse is true in the special cases $\mathbb{C}^2 \otimes \mathbb{C}^2$, and $\mathbb{C}^2 \otimes \mathbb{C}^3$ (Horodecki et al., 1996b).

There are also complete characterizations of entanglement in terms of *entanglement witness operators* and *positive maps* (Horodecki et al., 1996a), but their classifications turns out to be as complicate as the original problem of entangled mixed states.

¹¹Note that $\rho^{t,j} := \sum_{k=1}^r \lambda_k \rho_k^{(1)} \otimes \dots \otimes \rho_k^{(j),t} \otimes \dots \otimes \rho_k^{(n)} \geq 0$, since the coefficients and each factor matrix are non-negative, no matter which basis is chosen in \mathcal{H}_j to define the transpose.

B. Quantum Coding and Schumacher's Theorem

Let now $A := \{|\phi_i\rangle, p_i\}_{i=1}^{|A|}$ be a “quantum alphabet” consisting of a set of distinct pure states (not necessarily orthogonal) and their corresponding probabilities ($\sum_i p_i = 1$). We assign to it the following density operator $\rho(A) := \sum_i p_i |\phi_i\rangle\langle\phi_i|$. A message emitted by a source of quantum signals is now a sequence $\phi_{i_1 \dots i_n} := |\phi_{i_1}\rangle|\phi_{i_2}\rangle \dots |\phi_{i_n}\rangle$ of “quantum characters” or “quantum symbols”, each produced with probability p_{i_j} independently of the others. The collection of messages with n symbols is representable by the density operator $\rho^{\otimes n}$, which lives in a Hilbert space of maximum dimension $|A|^n = 2^{n \log_2 |A|}$. The question naturally arises again as to whether it is possible to compress the information contained in $\rho^{\otimes n}$. And the answer, found by Schumacher (Schumacher, 1995), is similar to Shannon's first theorem: asymptotically ($n \gg 1$) the state $\rho^{\otimes n}$ is compressible to a state in a Hilbert space of dimension $2^{nS(\rho)}$, with a *fidelity* F (probability that the decoded state coincides with the state prior to coding) arbitrarily close to 1. In other words, it is compressible to $nS(\rho)$ qubits. Then $S(\rho)$ can be thought of as the average number of qubits of essential quantum information, per character of the alphabet.

The idea of the proof follows the same guideline as for the classical theorem (Schumacher, 1995; Jozsa and Schumacher, 1994; Preskill, 1998). Let us diagonalize $\rho = \sum_r \lambda_r |r\rangle\langle r|$. The Von Neumann entropy $S(\rho)$ clearly coincides with the Shannon entropy $H(D)$ of the classical alphabet $D := \{r, \lambda_r\}_{r=1}^{|D|}$. Introducing the typical messages as those strings or tensor-product vectors $\psi_{i_1 \dots i_n} := |\psi_{i_1}\rangle \dots |\psi_{i_n}\rangle$ in the orthonormal basis that diagonalizes ρ , such that its probability $\lambda_{i_1 \dots i_n} := \prod_j \lambda_{i_j}$ satisfies $\lambda_{i_1 \dots i_n} \sim 2^{-nH(D)}$ for $n \gg 1$, it is shown that $\rho^{\otimes n}$ is asymptotically concentrated on the *typical subspace* T spanned by them: $\text{Tr}(P_T \rho^{\otimes n}) \sim 1$. Here P_T is the orthogonal projection onto T . The strategy of compression amounts to make a measurement that projects the original message $\phi_{i_1 \dots i_n}$ either onto T , or onto T^\perp . If the former is the case, the projected state $P_T \phi_{i_1 \dots i_n}$ is faithfully sent, upon coding it into $nH(D)$ qubits. What one does in the remaining case is irrelevant, for the probability that the result be $(1 - P_T)\phi_{i_1 \dots i_n}$ is asymptotically negligible.

The average fidelity in this procedure is perfect in the limit $n \rightarrow \infty$, and as in the classical theory, the quantum compression thus obtained is optimal.

If the alphabet $A := \{\rho_i, p_i\}_{i=1}^{|A|}$ is made up of mixed states, the issue of the message compressibility gets more involved. To properly measure it, the Shannon entropy $S(\rho := \sum_i p_i \rho_i)$ must yield to another more general concept, the so called *Holevo information* of the alphabet or ensemble $A := \{\rho_i, p_i\}_{i=1}^{|A|}$ (Levitin 1969; Holevo, 1973;

$$\chi(A) := S(\rho) - \sum_i p_i S(\rho_i). \quad (32)$$

The Holevo information is similar to the classical mutual information. As $I(X : Y)$ measures how the entropy of X gets reduced when Y is known, $\chi(A)$ represents the reduction of the entropy $S(\rho)$ of ρ , when the actual preparation of this state as a convex combination $\rho = \sum_i p_i \rho_i$ is known.

Assuming the states ρ_i of the alphabet to be mutually orthogonal, that is, $\text{Tr}(\rho_i \rho_j) = 0$ for $i \neq j$, it is not difficult to see that the state $\rho^{\otimes n}$ is asymptotically ($n \gg 1$) compressible to a state of $n\chi(A)$ qubits, with fidelity tending to 1. Moreover, this result is optimal.

When the states are not orthogonal, the results are only partial: it is known that there does not exist an asymptotically faithful compression below $\chi(A)$ per letter of the alphabet, but it is still open the problem of whether a compression of $\chi(A)$ qubits/character is or not accessible in the limit $n \rightarrow \infty$.

C. Capacities of a Quantum Channel

For a quantum transmission channel we can consider its capacity C for transmitting classical data, its capacity Q for transmitting quantum states exactly, and its mixed capacities $Q_{1,2}$ for transmitting quantum states, also exactly, but with the assistance of a classical side-channel between sender and receiver.

Given a quantum channel \mathcal{N} , usually noisy, Shannon's second theorem suggests to define the classical capacity $C(\mathcal{N})$ as the supremum of the transmission rates $R := k/n$ of classical words k -cbits long such that: 1/ Transmission is carried out after an appropriate word coding as n -bits words that are sent by n forward uses of the channel \mathcal{N} , followed by an associated decoding upon arrival (yielding words of k bits). 2/ The fidelity of the transmission is asymptotically 1. The quantum capacity $Q(\mathcal{N})$ is defined similarly by replacing the classical input/output words of k cbits by pure/mixed states of k qubits (Bennett and Shor, 1998).

The assisted quantum capacities $Q_{1,2}(\mathcal{N})$ are defined in a similar fashion as $Q(\mathcal{N})$, but now the coding-decoding protocol may include arbitrary local operations on input and output states, and may resort to a classical communication channel in the input-to-output direction (subscript 1), or in both directions (subscript 2).

It is possible to show that $Q = Q_1$ (Bennett et al. 1996; Bennett and Shor, 1998); that is, sending classical messages from origin to destination does not increase the channel capacity. On the other hand, it is evident that $Q \leq Q_2$, and using orthogonal states to transmit cbits leads to $Q \leq C$. But it is not known whether $C < Q_2$ holds or not. Channels are known for which $Q < Q_2$, and others for which $Q_2 < C$.

As asymptotically defined, it is not surprising that the computation of these capacities is usually difficult. In some instances they are known, as in the case of the so called *quantum erasure channel*, in which there is a probability p that the channel replaces the qubit by an erasure symbol orthogonal to the states $\{|0\rangle, |1\rangle\}$, and the complementary probability $1 - p$ that the qubit goes through exactly. For this type of channel $C = Q_2 = 1 - p$, and $Q = \max\{0, 1 - 2p\}$ (Bennett, DiVincenzo and Smolin, 1997; Bennett and Shor 1998).

Unlike the classical case, where the capacity can be computed maximizing the mutual information between input and output in a single use of the channel, the capacities (whether classical or quantum) of the quantum channels do not usually allow for a similar computation. This is because in this quantum case it is allowed to code by entangling several successive states on input, and to decode by means of joint measurements on several states on output. However, for the case C_{cq} (classical capacity with classical encoding and quantum decoding), it is known that $C_{\text{cq}}(\mathcal{N}) = \sup_{\rho} \chi(\mathcal{N}(\rho))$ (Bennett and Shor, 1998).

Finally, prior entanglement between sender and receiver improves the transmission capacity. Let C_E, Q_E be the classical and quantum entanglement-assisted capacities of a quantum channel. A direct consequence of the dense coding and quantum teleportation, to be described later, is the relation $C_E = 2C$ for noiseless quantum channels, and the relation $Q \leq Q_E = \frac{1}{2}C_E$ for any quantum channel (Bennett et al., 1999).

D. Quantum Error Correction

It is not possible in the quantum case just to plainly imitate the classical methods of error corrections, for merely trying to check which qubits have been affected by errors irremediably damages the information content. Neither can we make strings of equal quantum states, for the unitarity of quantum mechanics forbids the cloning of arbitrary unknown quantum states. This explains the initial pessimism about the possible functioning of a quantum computer (Landauer 1994; Unruh, 1995). Then, what to do? Fortunately enough, in 1995 Shor provided us with a first solution showing an encoding system (of 9:1 bits) capable of detecting and correcting one erroneous qubit.¹² Soon after, new and more economical codes were discovered, such as the 7:1 code of Steane (1996a; 1996b),

¹²Actually, the very first idea of quantum error correction, at the time called "recoherence", was proposed by Deutsch during his talk at the Rank Prize Funds Symposium on Quantum Communication and Cryptography (1993, Broadway, UK). This idea was later on developed further (Berthiaume, Deutsch and Jozsa, 1994; Barenco et al., 1997). Even the idea of decoherence free subspaces (Palma, Suominen and Ekert, 1996) preceded Shor's 9-qubit code.

Calderbank and Shor (1996), and the 5:1 code of Bennett et al. (1996).¹³ It is not possible to present here a full account of the many remarkable contributions in this field during the last six years. It is currently a developing field which, as it happened with the classical error correction codes, it has also been found unexpected connections with pure mathematics (Shor and Sloane, 1998).

The underlying idea of quantum error correction is to hide the information into subspaces of \mathbb{C}^{2^n} in order to protect it against decoherence and errors that only affect to a few qubits. To this end, if our system has k qubits (called “logical qubits”), a quantum error correction code (QECC) encodes their states by means of a linear isometric embedding $\pi : \mathbb{C}^{2^k} \hookrightarrow \mathbb{C}^{2^n}$, with $n > k$. We shall denote by \mathcal{Q} the image subspace of π , and its states will be called code states (or codewords). The additional $n - k$ qubits help us in protecting the information. The map π should disguise the information by delocalizing it, with the aim that errors (which often affect locally just one or a few qubits) may alter it nothing or the least possible (Preskill, 1998; Steane, 1997; Aharonov, 1998).

A system of n qubits in an initial pure state ψ is not absolutely isolated. Upon interaction with the environment in a state a_{in} , it suffers a transformation of the form $\psi \otimes a_{\text{in}} \mapsto \sum_r (E_r \psi) \otimes a_r$, where the operators E_r , $0 \leq r \leq 2^{2n} - 1$, are Pauli operators (elements of the set $\mathcal{P}^{(n)} := \{1, X, Y, Z\}^{\otimes n}$) and the environment states a_r are not necessarily orthogonal neither normalized. Let us call the *weight* of an element in $\mathcal{P}^{(n)}$ to the number of its nontrivial (i.e. X, Y, Z) tensor factors. If ψ is a code state, then each term $(E_r \psi) \otimes a_r$ represents a component with a number of errors equal to the weight of E_r .

Given a collection of errors $\mathcal{E} \subset \mathcal{P}^{(n)}$ formed by all the Pauli operators of weight $\leq t$, a QECC is said to amend up to t errors when it is capable of correcting every error in \mathcal{E} . For that to happen it is necessary and sufficient that $\langle \bar{j} | E_s^\dagger E_r | \bar{i} \rangle = m_{sr} \delta_{ji}$ be fulfilled, for any arbitrary orthonormal basis $\{|\bar{i}\rangle\}$ of the code subspace \mathcal{Q} and all $E_{r,s} \in \mathcal{E}$, m being a selfadjoint matrix. This condition means something quite natural: first, that given any two orthogonal codewords $|\bar{i}\rangle, |\bar{j}\rangle$, the sets $E_r |\bar{i}\rangle, E_r |\bar{j}\rangle$ of corrupted codewords must be mutually orthogonal, otherwise the perfect distinguishability of those words might get lost, and second, should $\langle \bar{i} | E_s^\dagger E_r | \bar{i} \rangle$ depend on $|\bar{i}\rangle$, the detection of the error would yield information about the code state, thereby perturbing it. If $m = \text{id}$, the code is called *nondegenerate*, and the error subspaces $E_r \mathcal{Q}$, $1 \neq E_r \in \mathcal{E}$ are orthogonal to the code subspace \mathcal{Q} and perpendicular one another. In this case it suffices to make a measurement, which is possible because of the orthogonality, that determines in which subspace the $(n$ -qubits system) \otimes environment lies. If the result of that measurement is $(E_r \psi) \otimes a_r$, by applying to the re-

sulting state of the system the unitary operator E_r^\dagger we shall retrieve the original state ψ free of error. In the degenerate case, an error syndrome does not singularize the error, and the retrieval strategy gets more involved.

The *distance* d of a QECC is defined as the lowest weight of a Pauli operator E such that $\langle \bar{j} | E | \bar{i} \rangle \neq c_E \delta_{ji}$. In analogy with the notation for CECCs, we shall write $[[n, k, d]]_2$ to denote a binary QECC (i.e., with qubits) of parameters n, k, d . It is easy to see that a code $[[n, k, d]]_2$ allows the correction of $t := \lfloor (d - 1)/2 \rfloor$ errors.

There are also asymptotic bounds for the QECCs $[[n, k, d]]_2$ similar to those presented for CCCEs (Ekert and Macchiavello, 1996; Preskill, 1998).

- Hamming’s quantum upper bound:

$$R := k/n \leq 1 - H_2(t/n) - (t/n) \log_2 3, \quad n \gg 1. \quad (33)$$

- Gilbert-Varshamov’ quantum lower bound:

$$R \geq 1 - H_2(2t/n) - (2t/n) \log_2 3, \quad n \gg 1. \quad (34)$$

As in the classical case, there exist QECCs which are asymptotically good. A different question (still open) is their explicit construction.

Example of QECC: CSS codes. Let \mathcal{C}_1 be a linear and binary CECC of type $[n, k_1, d_1]_2$, and $\mathcal{C}_2 \subset \mathcal{C}_1$ a subcode $[n, k_2, d_2]_2$ of \mathcal{C}_1 , with $k_2 < k_1$. Let $\mathcal{C} := \mathcal{C}_1/\mathcal{C}_2$ be the quotient space, of dimension $2^{k_1 - k_2}$.

Let us introduce a QECC $\mathcal{Q} \subset \mathbb{C}^{2^n}$ of dimension 2^k , with $k = k_1 - k_2$, spanned by the vectors

$$|\bar{w}\rangle := 2^{-k_2/2} \sum_{v \in \mathcal{C}_2} |w + v\rangle, \quad w \in \mathcal{C} \quad (35)$$

Note that this definition does not depend on the element w chosen to represent the class $w + \mathcal{C}$, and that the vectors $|\bar{w}\rangle$ thus constructed form an orthonormal system.

It can be shown that this quantum code recognizes and corrects (up to) $t_b := \lfloor (d_1 - 1)/2 \rfloor$ bit-flip errors X , and $t_{ph} := \lfloor (d_2^\perp - 1)/2 \rfloor$ phase-flip errors Z , where d_2^\perp is the distance of the code \mathcal{C}_2^\perp dual to \mathcal{C}_2 . Likewise, the distance d of this quantum code satisfies $d \geq \min(d_1, d_2^\perp)$.

The QECCs $[[n, k, d]]_2$ thus constructed are called CSS (Calderbank-Shor-Steane) codes (Steane, 1996a; Steane, 1996b; Calderbank and Shor, 1996; Preskill, 1998).

The simplest and most illustrative example of a CSS code is the $[[7, 1, 3]]_2$ code of Steane, or quantum code of 7 qubits. It is obtained taking as \mathcal{C}_1 the Hamming code $H_2(1)$ of type $[7, 4, 3]_2$, and as \mathcal{C}_2 its *dual* ($\mathcal{C}_2 = \mathcal{C}_1^\perp$), which is of type $[7, 3, 4]_2$, and coincides with the even subcode (that is, the code formed by the codewords of even weight)¹⁴ of \mathcal{C}_1 . It corrects one bit-flip error X , and

¹³An $n : 1$ code embeds 1 qubit into the space of n qubits.

¹⁴The weight of a binary word is defined as the number of its nonzero coordinates.

one phase-flip error Z . Thus, it also corrects a mixed error Y , but not a double bit-flip (or phase-flip) error.

A generator matrix for $H_2(1)$ is

$$G := \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (36)$$

and an associated parity matrix (generator for the dual) is

$$H := \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix} \quad (37)$$

Thus, a basis of code states is given by

$$\begin{aligned} |\bar{0}\rangle &:= 8^{-1/2}(|1010101\rangle + |0110011\rangle + \\ &\quad |0001111\rangle + |0000000\rangle + |1100110\rangle + \\ &\quad |1011010\rangle + |0111100\rangle + |1101001\rangle) \\ |\bar{1}\rangle &:= 8^{-1/2}(|0100101\rangle + |1000011\rangle + \\ &\quad |1111111\rangle + |1110000\rangle + |0010110\rangle + \\ &\quad |0101010\rangle + |1001100\rangle + |0011001\rangle) \end{aligned} \quad (38)$$

Let us assume that we have a qubit with a state coded as $|\bar{\phi}\rangle := \alpha|\bar{0}\rangle + \beta|\bar{1}\rangle$, in which a bit flip has occurred at the third place (X_3 error). How can we detect and correct it? With the help of an auxiliary system or *ancilla* A of $(n - k_1 = 3)$ -qubits long we form the state $(X_3|\bar{\phi}\rangle) \otimes |000\rangle_A$, which we transform by the unitary map defined on $\mathbb{C}^{2^n} \otimes \mathbb{C}^{2^3}$ by $|v\rangle \otimes |000\rangle_A \mapsto |v\rangle \otimes |He\rangle_A$, with the result $(X_3|\bar{\phi}\rangle) \otimes |He\rangle_A$, where $e := 0010000$ is the binary word that signals the place number 3 at which the bit-flip error occurred. But $He = 110$, which is also number 3 in (reversed) binary form. That is, we have marked in the ancilla the syndrome of the error made. It is essential that the ancilla remains in a state depending only on the error, and not on the particular state of the system. Now, it is enough to measure the state of the ancilla in order to find out that the error made has been X_3 , to apply the operator X_3^{-1} to the system in order to retrieve the state free of error $|\bar{\phi}\rangle$, and to bring back the ancilla to its neutral state $|000\rangle_A$. Finally suppose instead that the error to detect and correct is a phase flip at the fifth place (Z_5 error). Since $Z_5 = U_H^{\otimes 7} X_5 U_H^{\otimes 7}$, with U_H being the unary Hadamard application, it is enough for the system to go through the operation $U_H^{\otimes 7}$, to apply then the previous strategy, and finally to act with $U_H^{\otimes 7}$ once more.

E. Entanglement Distillation

In addition to quantum error-correction codes (QECC) there is another method to beat decoherence which is specially suitable when communicating over noisy channels.

It is based on the notion of *entanglement distillation* or *purification*: given two spatially separated parties A and B sharing a collection of entangled pairs, they are allowed to perform quantum local operations and classical communication (LOCC) (III.A) to extract a reduced sample of pairs with a higher purity of entanglement. Entanglement distillation serves as a useful tool for quantum communication providing us with more powerful protocols for dealing with errors (decoherence) than quantum error correction (Bennett et al., 1996a).

We need an *entanglement measure* (Vedral and Plenio, 1998). In distillation an appropriate entanglement measure for a pure bipartite state $|\Psi_{AB}\rangle$ is $E(|\Psi_{AB}\rangle)$ (27). The reason comes from the fact that given n pure bipartite states $|\Psi_{AB}\rangle$, local actions and classical communications are enough to prepare m perfect singlet states with a yield $\frac{m}{n}$ approaching $E(|\Psi_{AB}\rangle)$ as $n \rightarrow \infty$ (Bennett et al., 1996a; Bouwmeester, Ekert and Zeilinger, 2000).

Finding optimal purification procedures in full generality is open. However, explicit examples of *entanglement distillation protocols* EDP are known to work at least with particular types of mixed states, like the initial EDP introduced by Bennett et al. (1996a), which shall be referred as the *BBPSSW96 protocol*. It is neither optimal nor fully general, but it is the basic protocol known from which other generalizations are derived.

BBPSSW96 Protocol.

There are two parties A and B, Alice and Bob, which communicate over a noisy channel. They share entangled pairs of states and they aim at obtaining singlets (21) from them. Their basic strategy is to coordinate their actions through classical messages sacrificing some of the entangled pairs to increase the purity of the remaining ones.

Alice and Bob want to distill some pure entanglement, say in the form of singlet states $|\Psi^-\rangle$ (21), from a given collection of shared entangled pairs in an arbitrary bipartite mixed state ρ . The purity of ρ is measured through the fidelity

$$F := \langle \Psi^- | \rho | \Psi^- \rangle \quad (39)$$

relative to a perfect singlet.

To be specific, in this protocol Alice and Bob share two entangled pairs, each one in the state

$$\begin{aligned} W_F &:= F|\Psi^-\rangle\langle\Psi^-| + \\ &\quad \frac{1}{3}(1 - F)[|\Psi^+\rangle\langle\Psi^+| + |\Phi^+\rangle\langle\Phi^+| + |\Phi^-\rangle\langle\Phi^-|] \end{aligned} \quad (40)$$

These are called Werner states (1989). Note that they are depolarized in the space orthogonal to the singlet. The initial state in $(\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1}) \otimes (\mathcal{H}_{A_2} \otimes \mathcal{H}_{B_2})$ is therefore

$$\rho_0 := W_F \otimes W_F. \quad (41)$$

Before		After	
source	target	source	target
$ \Phi^\pm\rangle$	$ \Phi^\pm\rangle$	n.c.	n.c.
$ \Phi^\pm\rangle$	$ \Psi^\pm\rangle$	n.c.	n.c.
$ \Psi^\pm\rangle$	$ \Phi^\pm\rangle$	n.c.	$ \Psi^\pm\rangle$
$ \Psi^\pm\rangle$	$ \Psi^\pm\rangle$	n.c.	$ \Phi^\pm\rangle$
$ \Phi^\pm\rangle$	$ \Phi^\mp\rangle$	$ \Phi^\mp\rangle$	n.c.
$ \Phi^\pm\rangle$	$ \Psi^\mp\rangle$	$ \Phi^\mp\rangle$	n.c.
$ \Psi^\pm\rangle$	$ \Phi^\mp\rangle$	$ \Psi^\mp\rangle$	$ \Psi^\mp\rangle$
$ \Psi^\pm\rangle$	$ \Psi^\mp\rangle$	$ \Psi^\mp\rangle$	$ \Phi^\mp\rangle$

TABLE I: The two columns on the right list the states after the action of BCNOT (46) starting from the states on the left two columns. The notation is n.c.=no change.

We assume that the Werner pairs have fidelity $F > 1/2$. *Step 1.* Unilaterally, Alice (or Bob) applies the gate Y on each of her (his) two pairs of qubits. This brings ρ_0 to

$$\rho_1 := (Y \otimes 1) \otimes (Y \otimes 1) \rho_0 (Y \otimes 1) \otimes (Y \otimes 1) \quad (42)$$

The Pauli operators map the Bell states (21) onto one another in a 1:1 pairwise fashion, leaving no state unchanged (up to irrelevant phase factors which we will ignore); in particular $Y \otimes 1 : |\Psi^\pm\rangle \leftrightarrow |\Phi^\mp\rangle$. Then

$$\rho_1 = W'_F \otimes W'_F \quad (43)$$

with

$$W'_F := F|\Phi^+\rangle\langle\Phi^+| + \frac{1}{3}(1-F)[|\Phi^-\rangle\langle\Phi^-| + |\Psi^-\rangle\langle\Psi^-| + |\Psi^+\rangle\langle\Psi^+|] \quad (44)$$

The outcome is a new bipartite state with a large component $F > 1/2$ of $|\Phi^+\rangle$ and equal components of the other three Bell states.

Step 2. Bilaterally, Alice and Bob apply a CNOT operation (12) to each of their pairs of qubits. Let us denote this joint operation as U_{BCNOT} . Thus

$$\rho_1 \mapsto \rho_2 := U_{\text{BCNOT}} \rho_1 U_{\text{BCNOT}}. \quad (45)$$

This composite operation acts conditionally on qubits 3 and 4 (target qubits) depending on the states of qubits 1 and 2 (source qubits), namely

$$U_{\text{BCNOT}} := (|0\rangle\langle 0| \otimes 1 \otimes 1 \otimes 1 + |1\rangle\langle 1| \otimes 1 \otimes U_{\text{NOT}} \otimes 1) \cdot (1 \otimes |0\rangle\langle 0| \otimes 1 \otimes 1 + 1 \otimes |1\rangle\langle 1| \otimes 1 \otimes U_{\text{NOT}}) \quad (46)$$

The possible results of acting with BCNOT on the Bell states as source and target states are summarized in Table I.

Step 3. Alice and Bob measure (with respect to the computational basis) their target qubits, i.e., Alice measures

qubit 3 and Bob qubit 4. Then, they share their results by classical communication. If their results agree, they both keep their unmeasured source qubits, otherwise they discard them.

The source state ρ'_s thereby obtained is a convex combination of the Bell projections, with a weight of $|\Phi^+\rangle\langle\Phi^+|$ given by

$$F' := \frac{F^2 + \frac{1}{9}(1-F)^2}{F^2 + \frac{2}{3}F(1-F) + \frac{5}{9}(1-F)^2}. \quad (47)$$

The rest $1-F'$ is not equally distributed among the other three Bell states.

Step 4. Unilaterally, Alice (or Bob) applies Y on her (his) source qubit in order to convert ρ'_s into a state ρ_s of fidelity F' (relative to $|\Psi^-\rangle$).

Step 5. The state ρ_s is not a Werner state. But there is a depolarizing procedure, called bilateral random operation, which mutates it back into a such one while preserving its fidelity (Bennett et al., 1996b).

The net result of this protocol is that with probability greater than $\frac{1}{4}$, one Werner pair of fidelity $F' > F > \frac{1}{2}$ (47) is distilled out of two Werner pairs of fidelity $F > \frac{1}{2}$.

An initial supply of N Werner states of fidelity F is halved by a single run of the above protocol to a sample of Werner states of fidelity $F' > F$. Iterating the procedure as much as necessary, Werner states of purity F_{out} arbitrarily close to 1 can be distilled from a supply of input mixed states ρ of any purity $F_{\text{in}} > \frac{1}{2}$.¹⁵

The overall result of the BBPSSW96 protocol is to simulate a noiseless quantum channel by a noisy one assisted with local actions and classical communication (LOCC). It assumes tacitly that the quantum channel is shorter than its coherence length; otherwise one may resort to the assistance of *quantum repeaters* (Dür et al. 1999).

There exist also EDP protocols using one single pair of qubits (Gisin, 1996; Kwiat et al., 2001).

Finding the optimal distillation protocols for a general state and any number of copies is the unsolved *distillability problem*. Despite this lack of knowledge, a surprising result is the existence of entangled states that cannot be distilled and are called *bound entangled* (Horodecki et al., 1998). Explicit examples of entangled mixed states of two qutrits that cannot be distilled were found by Horodecki et al. (1999). These states are useless for quantum communication protocols and it is important to distinguish them from distillable states that are also called *free entangled*. In some general instances, it is possible to conclude that a mixed state is bound entangled: if ρ is entangled and satisfies the Peres criterion $\rho^{t,j} \geq 0$ (Sec. III.A) then ρ is a bound entangled state (Horodecki et al., 1998).

¹⁵The map $F \mapsto F'$ is strictly increasing in the interval $[\frac{1}{2}, 1]$, and has an attractive fixed point at $F = 1$.

In summary, entanglement is a new resource for computation processing and communication that can change information theory both qualitatively and quantitatively. The concept of entanglement is a genuinely quantum phenomenon that allows us to extend the theory of information beyond its classical limitations. We have already seen error-correction codes as one essential application of entanglement and more genuine examples like teleportation, dense coding, quantum key distribution, quantum computations, etc. are addressed in the forthcoming sections.

IV. QUANTUM TELEPORTATION

Copying classical states (be it an Etruscan fibula, a Goya painting, or a banknote) has never posed unsurmountable difficulties to experts. It suffices to thoroughly observe the original as much as it may be required, taking care of not damaging it, to retrieve the information needed to make a copy of it. This careful observation does not alter in a noticeable way its state. But if the original to be reproduced is a quantum system in an unknown state ϕ , then any measurement (incompatible with P_ϕ) made on the system to get information on ϕ will perturb uncontrollably the state destroying the original (Sec. III). Moreover, even having an unlimited number of copies of that state, infinitely many measurements will be necessary to determine that unknown state.

For example, let us assume that Alice has a qubit (say one spin $\frac{1}{2}$) in a pure state. Bob needs it, but Alice does not have any quantum channel to transmit it to him. If Alice knows the precise state of her qubit (for example, if she knows that her spin $\frac{1}{2}$ is oriented in the direction \mathbf{n}), it is enough for her to give Bob in a letter (classical channel) that information (the components of \mathbf{n}) to enable him preparing a qubit exactly equal to Alice's. But if she happens not to know the state, she may choose to confess it to Bob, who would then be inevitably driven to prepare his qubit in a random way, obtaining a 50% fidelity on average. But Alice can also try to be more cooperative, making for example a measurement on her qubit of $\mathbf{n} \cdot \boldsymbol{\sigma}$, with \mathbf{n} arbitrarily chosen, and then transmitting to Bob both the components of \mathbf{n} and the result $\epsilon = \pm 1$ thus obtained. Armed with this information, Bob can prepare his qubit in the state $\frac{1}{2}(1 + \epsilon \mathbf{n} \cdot \boldsymbol{\sigma})$. The average fidelity so obtained is larger than before: $2/3$. However, it is not enough.

If Alice and Bob share an EPR pair, there exists a protocol, devised by Bennett et al. (1993), known as *quantum teleportation*, which resorting to the quantum entanglement of states and the non-locality of quantum mechanics, it allows Bob to reproduce Alice's unknown quantum state with the assistance of only 2 cbits of information sent by Alice to Bob through a classical channel. This procedure necessarily destroys Alice's state (otherwise it would violate the quantum no-cloning theorem,

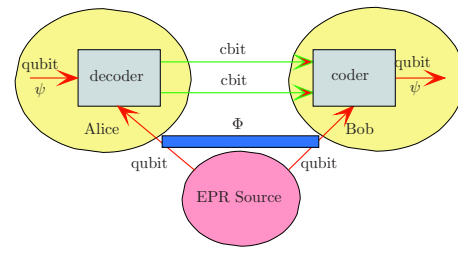


FIG. 3: Scheme for quantum teleportation.

Sec. III). Let us have a closer look at the aforementioned protocol (see Fig.3) (Rieffel and Polack, 1998).

Let $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ be Alice's qubit, with $\alpha = \cos \frac{1}{2}\theta$, $\beta = e^{i\phi} \sin \frac{1}{2}\theta$. And let $|\Phi\rangle := 2^{-1/2}(|00\rangle + |11\rangle)$ be the EPR state shared by Alice and Bob, with Alice having the first of its qubits, and Bob the second. The initial state is thus $|\psi\rangle \otimes |\Phi\rangle$, of which Alice can locally manipulate its two first bits and Bob the third one.

Step 1. Alice applies to the initial state the unitary operator $U := ((U_H \otimes 1)U_{\text{CNOT}}) \otimes 1$, acting with the CNOT gate on the first two qubits and next with the Hadamard gate H on the first one. The resulting state is

$$\frac{1}{2}(|00\rangle \otimes |\psi\rangle + |01\rangle \otimes X|\psi\rangle + |10\rangle \otimes Z|\psi\rangle + |11\rangle \otimes Y|\psi\rangle). \quad (48)$$

Step 2. Alice then measures the first two qubits, obtaining $|00\rangle, |01\rangle, |10\rangle$, or $|11\rangle$ equiprobably.¹⁶ Alice lets Bob know the result thus obtained, sending him two cbits: the pair of binary digits 00, 01, 10, 11 that characterizes it. As a byproduct of Alice's measurement, the first bit ceases to be in the original state $|\psi\rangle$, while the third qubit gets projected onto $|\psi\rangle, X|\psi\rangle, Z|\psi\rangle, Y|\psi\rangle$, respectively.

And step 3. Once Bob receives the classical information sent by Alice, he just needs to apply on his qubit the corresponding gate 1, X, Z, Y, in order to drive it to the desired state $|\psi\rangle$.

Notice that this teleportation sends an unknown quantum state from one place (whence it vanishes) to another place (where it shows up) without really traversing the intermediate space. It does not violate causality, though. In the first part of the process, quantum correlations get established between the Bell states obtained by Alice and the associated states of Bob's qubit. In the remaining part to conclude the teleportation, information is transmitted by classical means, in the standard

¹⁶Steps 1+2 amount to performing a Bell measurement on the initial state, thus correlating the Bell states $00 \pm 11, 01 \pm 10$ of Alice's two qubits with the states of Bob's qubit. It suffices to note that

$$|\psi\rangle|\Phi\rangle = \frac{1}{\sqrt{2}}|\psi\rangle(|00\rangle + |11\rangle) = \frac{1}{2\sqrt{2}}((|00\rangle + |11\rangle)|\psi\rangle + (|01\rangle + |10\rangle)X|\psi\rangle + (|00\rangle - |11\rangle)Z|\psi\rangle + (|01\rangle - |10\rangle)Y|\psi\rangle).$$

non-superluminal fashion. Notice also that in this “non-corporeal” process, it is the information about the quantum state, the qubit, and not the physical state itself, what gets passed from Alice to Bob. There has been no transportation whatsoever of matter, energy or information at a speed larger than the speed of light.

It is nevertheless surprising in the quantum teleportation that all the information needed to reproduce the state $|\psi\rangle = (\cos \frac{1}{2}\theta)|0\rangle + e^{i\phi}(\sin \frac{1}{2}\theta)|1\rangle$ (information that is infinite for it requires to fix a point (θ, ϕ) on the Bloch sphere with infinite precision, thus requiring infinitely many qubits), can be accomplished with only 2 cbits, provided an EPR state is shared. This state, by itself, only generates potentially an infinite number of random and correlated bit pairs.

An *ebit* is the amount of entanglement in a two-qubit state maximally entangled (usually, in a bipartite pure state with entanglement entropy 1) (Bennett et al., 1996). As an “exchange currency”, one ebit is a computing resource made up of a shared EPR pair. Writing $a \triangleleft b$ to indicate that a resource a is implementable upon spending the resource b , the following relations are quite apparent: 1 cbit \triangleleft 1 qubit (to transmit 1 cbit it is enough to send 1 qubit in one out of two orthogonal states), 1 ebit \triangleleft 1 qubit (to have 1 ebit it is enough to produce an EPR pair and to send one half of it to the other partner). With this formulation, the quantum teleportation allows us to write: 1 qbit \triangleleft 1 ebit + 2 cbits (Bennett, 1995a).

Quantum teleportation was realized experimentally with photons for the first time in two laboratories (Bouwmeester et al., 1997; Boschi et al., 1998). This is at least what these authors claim, although several critiques have been raised (Braunstein and Kimble, 1998; Vaidman, 1998; Braunstein, Fuchs and Kimble, 1999) (see however Bouwmeester et al. (1998; 1999)). In the experiment by the Roma group (Boschi et al., 1998), the initial state to be teleported from Alice to Bob was a photon polarization, but not an arbitrary one, for it coincided with that of the Alice’s photon in the shared EPR photon pair. In the experiments by the Innsbruck group (Bouwmeester et al., 1997), however, the teleported state was arbitrary. Teleportation was reached with a high fidelity of 0.80 ± 0.05 ,¹⁷ but with a reduced efficiency (a 25% of cases).

It does not seem to be easy to implement the theoretical protocol with a 100% effectiveness. The Bell operator (which distinguishes among the four Bell states of 2 qubits) cannot be measured unless both qubits interact appreciably one each other (as it occurs with the CNOT gate used in the protocol explained above), something which is very hard to achieve with photons. However, with atoms in EM cavities the hopes are high.

¹⁷This fidelity overcomes the value $\frac{2}{3}$ corresponding to the case in which Alice measures her qubit and communicates the result to Bob classically.

Teleportation has also been realized of states which are parts of entangled states (Pan et al., 1998).

It is also worthwhile mentioning quantum teleportation of states of infinite dimensional systems (Furuzawa et al., 1998), namely, the teleportation of coherent optical states leaning on pairs of EPR squeezed states. In this experiment, whose fidelity is 0.58 ± 0.02 (higher than the maximum $\frac{1}{2}$ expected without resorting to entanglement), a third party, the *verifier* Victor, supplies Alice with one state that is known to him, but not to her. After teleporting that state from Alice to Bob, Victor verifies on output if Bob’s state is similar to the one he provided to Alice. In this sense, this experiment is different from all the others, and led the authors to claim priority in the realization of teleporting.

Quantum teleportation, which doubtlessly will be extended to entangled states from different kinds of systems (photons and atoms, ions and phonons, etc.), might have in the future remarkable applications for quantum computers and in computer networks (for example, combined with prior distillation of good EPR pairs), as well as in the production of quantum memory records by means of teleportation of information on systems such as photons to other systems as trapped, well-isolated ions in cavities (Bennett, 1995a; Bouwmeester et al, 1997).

V. DENSE CODING

Classical information can also be sent through quantum channels: to transmit the word 10011, it is enough that Alice prepares 5 qubits in the states $|1\rangle, |0\rangle, |0\rangle, |1\rangle, |1\rangle$, sends them to Bob through the quantum channel, and Bob measures each of them in the basis $\{|0\rangle, |1\rangle\}$. Each qubit carries a cbit, and this is the most it can do in isolation. But if Alice and Bob share beforehand an entangled state, then 2 cbits of information can be sent from Alice to Bob with a single qubit. This is cast in the formula: 2 cbits \triangleleft 1 ebit + 1 qubit.

As a matter of fact, entanglement is a computing resource that allows more efficient ways of coding information (Bennett and Wiesner, 1992). One of them goes under the name of *quantum dense coding* (or superdense coding). Assume, for instance, an entangled state of two photons. One of the photons goes to Alice, the other one to Bob. She performs one of the following operations on the polarization of her arriving photon: identity, flipping (that is, \leftrightarrow , $\uparrow \rightleftharpoons \downarrow$, or $\circ \rightleftharpoons \odot$), change of π in the relative phase, and the product of the last two. Once this is done, she sends back the photon to Bob, who measures in which of the four Bell states the photon pair is. Then, in this fashion we have been able to send 2 bits of information over one single particle with only 2 states, that is, by means of a qubit. It doubles what can be accomplished classically. Thereby the name of dense coding. Moreover, if Eve intercepts the qubit, she cannot get from it alone any information whatsoever for its state is $\frac{1}{2}I$. All the information lies in the entangled state, and Bob possesses

half of the pair. Actually, Alice has sent Bob 2 qubits, but the first one long ago, as part of the initial entangled state. This fact has allowed them to communicate more efficiently, resorting to the entangled state they shared.

Dense coding is kind of the inverse process to teleportation. In the latter the communication of two cbits allows us to reproduce a qubit state, while in the former the communication of a qubit carries along two cbits of information.

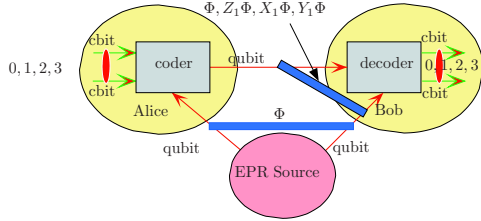


FIG. 4: Scheme for dense quantum coding.

The following is a protocol that thoroughly implements what we have just explained (Rieffel and Polack, 1998): an EPR source supplies Alice and Bob with EPR two-particle states like $|\Phi\rangle := 2^{-1/2}(|00\rangle + |11\rangle)$, one of whose particles goes to Alice and the other one to Bob, who keep them. Alice is supplied with 2 cbits, which represent the numbers 0, 1, 2, 3 as 00, 01, 10, 11 (see figure 4).

Step 1. Coding. According to the value of that number, Alice effects on her EPR half the unitary operation 1, Z , X , Y , which brings the EPR state to 00+11, 00-11, 10+01, 10-01. Once this is done, she sends her half to Bob.

Step 2. Decoding. Upon reception, Bob effects on the EPR pair first a CNOT operation, such that the state becomes 00+10, 00-10, 11+01, 11-01. He then measures the second qubit; if he finds 0, he already knows that the message was 0 or 1, and if he finds 1, the message was 2 or 3. That is, he has gotten the first bit of the two-bit message. In order to know the second one, Bob next applies a Hadamard transformation on the first qubit, thereby the state becomes 00, 10, 01, -11, and measuring the first bit, if he finds 0, he knows that the message was 0 or 2, and if he finds 1, the message was 1 or 3, that is, he has just gotten the second bit of the message.

An experiment of this nature has been performed in Innsbruck (Mattle et al., 1996), using as a source of entangled photons the parametric down conversion that a non-linear crystal of β -barium borate produces: UV photons get disintegrated (though with low probability) in a pair of softer photons, with polarizations which in a certain geometric configuration they are entangled. In that experiment it was achieved to send 1 qutrit/qubit, that is, $\log_2 3 = 1.58$ cbits per qubit.

In a recent experiment, in which the qubits are the spins of ^1H y ^{13}C in a chlorophorm molecule $^{13}\text{CHCl}_3$ marked with ^{13}C , and RMN techniques are employed to

initialize, manipulate and read out the spins, the authors claim to have reached the 2 cbits per qubit (Fang et al., 1999).

The initial preparation of the entangled pair and the posterior transmission of the information qubit may have opposite senses; for example, Bob sends to Alice one half of the entangled state, keeping the other half for himself, and then Alice uses her qubit to send to Bob the desired information. This may be of interest if the cost in the transmission in one way is higher than in the reverse way. Being the distribution of the entangled state prior to the communication, transmission hours at lower charges can be profited from.

On the other hand, intercepting the message from Alice to Bob does not provide a trifle of information to an eavesdropper, for the message is entangled with the part of the EPR system possessed by Bob. Therefore it is automatically an encrypted emission (except if Eve intercepts both the original pair and the message and she replaces them).

VI. CRYPTOGRAPHY

A. Classical Cryptography

Cryptography is a very important part of information theory since 1949, with the pioneering works by Shannon at Bell Labs. He proved that there exist unbreakable codes or *perfectly secret* systems (Shannon, 1949). As a matter of fact, one was known since 1918 (but not that it were unbreakable): the *one-time pad* system (ONETIMEPAD). It is also named VERNAM code (Vernam, 1926), for it was devised by the young engineer Vernam at AT&T in December 1917 and proposed to the company in 1918 (Kahn, 1967); with Vernam's system both ciphering and deciphering of messages became automatic tasks for the first time.

1. One-time pad

To encode with the one-time pad one starts from the *plain* or *source* text to be ciphered, written as a series $\{p_1, p_2, \dots, p_N\}$ of integers $p_j \in \mathbb{Z}_B$; then a *key* $\{k_1, k_2, \dots, k_M\} \in \mathbb{Z}_B^M$, $M \geq N$, randomly chosen, is used to produce a *ciphered* text or *cryptogram* $\{c_1, c_2, \dots, c_N\}$ by combining the key with the plain text in modular arithmetic $c_j := p_j + k_j \bmod B$, $1 \leq j \leq N$. The module B is the maximum number of distinct symbols (2 for binary, 10 for digits, 27 for letters (English text and blank space symbol), etc.).

Both the sender (Alice) and the receiver (Bob) need to have the same key of random numbers, so that upon reception of the cryptogram, Bob undoes the algorithm with that key recovering thereby the original text.

Possible repetitions in the source text (to which codebreakers resort for decoding) are washed out by the random key. The length of the random sequence must be greater than or equal to that of the source text, and must not be employed more than once.¹⁸ Shannon showed that if the key length is smaller than the text length and one reuses cyclically the key to encrypt the message, then it is possible to extract information from the encoded text (Shannon, 1949). These requirements make this procedure very burdensome when there are lots of information to encrypt. Moreover, it is not easy to have long series of really random numbers at our disposal.

This cipher system was used by German and Russian diplomats during the Second World War, and by the soviet espionage during the cold war (Hughes et al., 1995). It is popularly known as “one-time pad” because the keys were written on a notebook or pad, and each time one was used, the corresponding sheet with the key was torn off and destroyed. It is said that the continued use of the same key allowed to unmask the Rosenberg spy ring and the atom-spy Fuchs (Hughes et al., 1995). It was also used by Che Guevara to communicate secretly with Fidel Castro from Bolivia (Bennett, Brassard and Ekert, 1992). And it is routinely used for White House and Kremlin communications through the “hot line”.

Although invulnerable, the VERNAM cryptosystem has the shortcoming of demanding keys so long at least as the text to be ciphered. This is why it is only used to cipher highly valuable information. For less delicate or sensitive business it is replaced by shorter though breakable encryption keys.

It was precisely the spur for breaking secret messages what fostered the development of computers.

2. PKC System

The PKC system (*Public Key Cryptographic System*) is of great interest since it avoids some of the shortcomings of the VERNAM system. It was devised in the middle of the 70s by Diffie and Hellman at Stanford (Diffie and Hellman, 1976; Diffie, 1992; Hellman, 1979) and later implemented at MIT by Rivest, Shamir and Adleman (1978).¹⁹ This system is nowadays used worldwide, for instance in Internet.

Two keys are involved: one person X gives away a public key, which anybody can use, and he/she keeps secret a private key, which is the inverse of the former. The public key is used by any sender S to send coded messages

¹⁸If two binary cryptograms encoded with the same key are intercepted, their sum modulo 2 eliminates the key and makes it possible to decrypt messages with certain ease (Collings, 1992).

¹⁹Apparently, some years before Diffie and Hellman, the British Secret Service knew about this system, but as classified record (military secret) (Ellis, 1970; Ekert, Hayden and Inamori, 2000).

to X ; on receipt, X decodes them with the private key. It is pretty clear that this is of interest only if X alone, but nobody else, knows how to undo the coding at a reasonable cost. How can we get this done? In a subtle and cunning way: to encrypt messages, the PKC system uses trapdoor one-way functions. These are injective maps of complexity \mathbf{P} , i.e., (computationally) *tractable* functions, the inverses of which are *untractable* in practice, that is, high costly to evaluate unless additional information is supplied (\mathbf{NP} problem). See Appendix for details. Integer factorization stands out among this type of inverse functions, as well as discrete logarithms in finite fields and on elliptic curves (Koblitz, 1994; Welsh, 1995).

The PKC system affords to leave wide open both the encryption algorithm and “half” of the total key, namely the public key, without suffering from any extra insecurity; this contrasts sharply with the controversial DES system (*Data Encryption Standard*), which discloses only the algorithm, but whose vulnerability has been shown up (Electronic Frontier Foundation, 1998).

3. RSA System

One of the most interesting ways of implementing the PKC system is the RSA method of Rivest, Shamir, and Adleman, 1978, based on the extreme difficulty of factoring large integer numbers. In particular, it is used to protect the electronic bank accounts (for instance, against bank transfers electronically requested). The public key of X consists of a pair of integers $(N(X), c(X))$, the first one very big, say of 200-300 digits, and the other one in the interval $(1, \varphi(N(X)))$ and coprime to $\varphi(N(X))$, where φ is Euler’s totient function ($\varphi(n)$ is the number of coprimes to n in the interval $[0, n)$). Upon transforming the sender S his/her message M into an integer following some public bijective prescription which both sender and receiver have agreed upon, he/she partitions it into blocks $B_j < N(X)$ as lengthy as possible, encodes each block B as

$$B \mapsto C(B) \equiv B^{c(X)} \bmod N(X), \quad (49)$$

and sends the sequence of *cryptograms* $\{C(B_j)\}$ to X . Let us denote this coding operation as $M \mapsto P_X(M)$, with the symbol P_X meaning that it was done with the *public key* $c(X)$ of X . The receiver X decodes each $C(B)$ as

$$C(B) \mapsto B \equiv C(B)^{d(X)} \bmod N(X), \quad (50)$$

where the exponent $d(X)$ for decoding is the *private key*, which is nothing but a solution to

$$c(X)d(X) \equiv 1 \bmod \varphi(N(X)). \quad (51)$$

That solution is (Koblitz, 1994)

$$d(X) \equiv c(X)^{\varphi(N(X))-1} \bmod \varphi(N(X)). \quad (52)$$

We shall indicate the decoding as $P_X(M) \mapsto S_X(P_X(M)) = M$, where the symbol S_X refers to the secret key of X .

In principle, since $c(X)$ and $N(X)$ are known, anybody can compute $d(X)$, and hence break up the secret. But it is here where the shrewdness of X enters the stage. In order to make it extremely difficult to Eve (spy character that intercepts messages, and listens to them without permission before delivering them again), it is better that X abides by certain rules (Salomaa, 1996), among which we highlight the following:

1. He/she must choose $N(X)$ as the product p_1, p_2 of two large and random prime numbers (with at least one hundred digits each), not very close one another (for this it is enough that the lengths of their expressions differ in a few bits), and avoiding also that they be tabulated or have some special form. Algorithms for testing primality like the probabilistic algorithm of Miller-Rabin (Miller, 1980; Rabin, 1976), or the deterministic APRCL, discovered by Adleman, Pomerance, and Rumely (1983), and later simplified and improved by Lenstra and Cohen (Cohen and Lenstra 1984; Cohen, 1993) facilitate enormously the election of p_1, p_2 .
2. As X knows p_1, p_2 , he/she knows how to compute $\varphi(N(X))$, namely, $\varphi(N(X)) = (p_1 - 1)(p_2 - 1)$. Now X has to choose an integer $d(X)$ (the private key) randomly in the interval $(1, \varphi(N(X)))$, coprime to $\varphi(N(X))$, and then compute the public key $c(X)$ by means of

$$c(X) \equiv d(X)^{\varphi(N(X))^{-1}} \bmod \varphi(N(X)), \quad (53)$$

or, much better, by solving $c(X)d(X) \equiv 1 \bmod \varphi(N(X))$ with the classical Euclid's algorithm.

One should discard small private keys $d(X)$, in order to avoid their disclosure by plain trial and error. That is why it is convenient to start by fixing $d(X)$. It is not advisable to have $c(X)$ very small either, for then the interception of the same message sent to several addressees sharing the same public key could lead to its break-up without much effort.

Anybody knowing only $N(X)$ but not its factors, should "apparently" factorize first $N(X)$ to compute $\varphi(N(X))$, and hence to find out the exponent for decoding;²⁰ but factorization of a number 250 digits long would take about 10 million years on a 200 MIPS²¹ workstation with the best algorithm known nowadays (Hughes, 1997).

²⁰"Apparently", for it is unknown so far whether there exist alternative procedures to decode $C(B)$ which do not go through getting the inverse exponent, nor whether the computation of this one necessarily requires to know the prime factors of N .

²¹Million of instructions per second; it gives a general idea of a computer's speed, but only refers to CPU speed (real speed depends also on other factors like input/output speed).

The RSA system also allows digital *authentication* of messages, as well as appending to them an *electronic* or *digital signature* (van der Lubbe, 1998; Koblitz, 1994; Stinson, 1995; Welsh, 1995).

a. The RSA numbers.

In 1977 Martin Gardner published an encoded message in his MATHEMATICAL GAMES of Scientific American using the RSA method, with the promise of a \$ 100 reward (payable by the Rivest *et al.* group at MIT) for the first person who would decode it (Gardner, 1977):

96869613754622061477140922254355882905759991124
57431987469512093081629822514570835693147662288
3989628013391990551829945157815154

This cryptomessage had been obtained using the RSA method starting from an English sentence and the dictionary \square (blank space) $\mapsto 00$, $a \mapsto 01, \dots, z \mapsto 26$), and using as public key (RSA-129, 9007), where RSA-129 was the following number 129 digits long:

RSA-129 = 114381625757888867669235779976146612
01021829672124236256256184293570693524573389783
0597123563958705058989075147599290026879543541

Decoding this message required to factorize RSA-129 into two prime factors of 64 and 65 digits each. It was estimated by then that the time to reach that goal would be about 4×10^{16} years, at least. In 1994 new factorization algorithms²² and the combined effort in idle time of a cluster of about a thousand workstations on the Internet did factorize it in about 8 months, after a CPU time of 5000 MIPS years, using the quadratic sieve algorithm (QS). These factors are

34905295108476509491478496199038981334177646384
93387843990820577 x
32769132993266709549961988190834461413177642967
992942539798288533

With this knowledge, it is straightforward to recover the original message: **the magic words are squeamish ossifrage** (Atkins, 1995).

²²There exist efficient methods, like those based on the quadratic sieve (QS) (Pomerance, 1982; Gerber, 1983; Pomerance, 1996), elliptic curves (EC) (Lenstra, 1987), and the general number field sieve (GNFS) (Lenstra, 1993; Pomerance, 1996). Their complexities are subexponential, but superpolynomial:

$$\text{QS: } \mathcal{O}(e^{(1+o(1))\sqrt{\log N \log \log N}})$$

$$\text{EC: } \mathcal{O}(e^{(1+o(1))\sqrt{\log p \log \log p}})$$

$$\text{GNFS: } \mathcal{O}(e^{(1.923+o(1))(\log N)^{1/3}(\log \log N)^{2/3}})$$

where p is the smallest prime factor of N . From 120-130 digits on, the number field sieve seems to overcome the other methods.

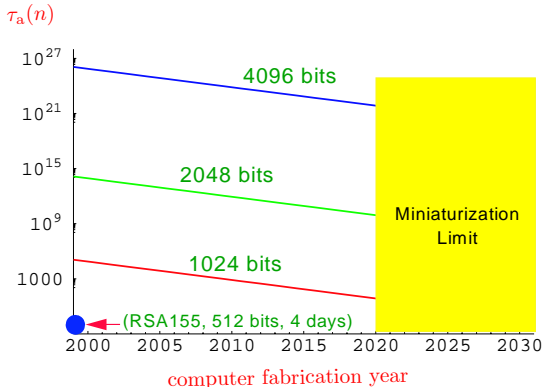


FIG. 5: Factorization with 1000 workstations with increasing power according to Moore’s law starting from 800 MIPS in 2000. The vertical axis shows the factorization time $\tau_a(n)$, in years, for an integer number of n bits. The horizontal axis shows the calendar year.

Two years later, RSA-130 was broken with the most powerful factorization algorithm till date (the general number field sieve (GNFS)), and after a computation time almost one order of magnitude lower than that employed for RSA-129. In February 1999, the factorization of the next number in the RSA list was over: the RSA-140, after about 2000 MPIS-years and the same GNFS method. And in August 1999 the factorization of RSA-155 was achieved, also using GNFS and after about 8000 MIPS-years.²³ It has 512 bits and is the product of two prime numbers 78 digits long. Just to figure out the magnitude of this problem, in its solution 35.7 CPU years have been employed to do the sieve, distributed in about three hundred workstations and PC’s, and 224 CPU hours of CRAY C916 and 2 Gbytes of central memory in order to find the relations between the rows of a giant sparse matrix of 6.7 million rows and as many columns, with an average of 62.27 non-vanishing elements per row.

A few years ago, it was considered as very safe the usage of 512-bits modules.²⁴ The preceeding example shows that the GNFS factorization algorithm renders this bit length insufficient. Nowadays, the use of (768, 1024, 2048)-bits modules is recommended for (personal, corporate, highly security)-use. In Fig. 5, the estimated factorization times under the joint use of 1000 workstations is represented, assuming that the processing power follows the so called *Moore’s law* (doubling every 18 months) (Hughes, 1997). See Sec. VII for more details. We take the RSA-155 time as reference.²⁵

²³We thank A.K. Lenstra and H.te.Riele for sharing with us their information about the latest RSA’s factorizations.

²⁴The number of bits in the integer N is $\lfloor \log_2 N \rfloor + 1$.

²⁵Miniaturization of classical devices has the atomic/molecular scale as a limit, which at Moore law’s pace will be reached within

Even though the factorization problem remains as a hard problem in computer science, nobody knows for sure whether one day a mathematician may come up with a radically new faster algorithm such that the ordinary classical computers can cope with the task of factorizing large integer numbers in polynomial time. As a matter of fact, quantum computation has raised high expectations in this regard, with Shor’s algorithm (Shor, 1994) to be discussed in Sec. X.D. That is why security agencies closely follow the new advances in number theory and computation to see what they are up to!

B. Quantum Cryptography

Quantum physics provide us with a secure method for coding, guaranteed by the very laws of physics. The pioneering idea dates back to Stephen Wiesner, who already by 1969²⁶ suggested this possibility, as well as the fabrication of forgery-proof banknotes, *quantum* banknotes (Wiesner, 1983). In the middle ’80s Bennett and Brassard (1984) devised a quantum cryptosystem based on the Heisenberg principle, which soon afterwards was implemented experimentally by sending secret information with polarized photons to a distance 30 cm apart (Bennett et al., 1992). This system employs quantum states, not all mutually orthogonal, in order to keep them from being cloned by a possible interceptor; as it uses 4 distinct states, it is coined the *four-state scheme*. Using non-local quantum correlations in pairs of entangled photons (produced, for example, by parametric down conversion) was subsequently proposed by Ekert (1991). Within this E91 system the Bell inequalities (Bell, 1964; 1966; 1987) are in charge of keeping the security; hence this system is also labeled *EPR scheme*. For a detailed recent review see Gisin et al., 2001.

1. Counterfeit-safe “quantum” banknotes

A possible forger-proof banknote could be a banknote provided with a printed number and a small collection of (say twenty) photons trapped indefinitely in individual cells of perfectly reflecting walls, and with secret polarizations $\odot, \oslash, \uparrow, \leftrightarrow$ randomly distributed, that the issuing bank would keep in secret correspondence with the identification number. The bank therefore could at any moment check the legitimacy of the note, without ruining it, because it would know beforehand how to place the polarizers to check each photon polarization without destroying it. Any forger that attempts to copy a note, however,

a couple of decades.

²⁶His work was finally published in 1983, but after being rejected from the journal to which it was first submitted. An unpublished version appeared in 1970.

ignorant of the directions in which the photons were polarized, would perturb the initial polarization projecting it onto some of two corresponding orientations of the polarizer chosen to measure with (Wiesner, 1983; Bennett, 1992b).



FIG. 6: Counterfeit-safe banknotes: the identification number is correlated with the secret polarizations of photons trapped in individual cells.

2. QKD: quantum key distribution

Although the quantum notes business may look a seer fantasy, this is not the case for systems of quantum key distribution. Among the communication protocols, we may highlight the BB84 of Bennett and Brassard (1984), E91 of Ekert (1991), B92 of Bennett (1992a), and EPR without Bell's inequalities, due to Bennett, Brassard and Mermin (1992). These protocols provide a way for two parties to share keys absolutely secret in principle, and thus they are an ideal complement to the Vernam code.

Alice and Bob want to exchange secret information, without recourse to middlemen who bring key pads from one to the other, and without fear that someone breaks their code. To this end, they must share a key, known only to them. They proceed according to a given communication *protocol*, or set of instructions either to detect any non-authorized eavesdropper, or else to settle down the secret key that only they will share for coding and decoding.

a. BB84 Protocol, or four-state scheme.

This is the first protocol devised in quantum cryptography. Alice and Bob are connected by two channels, one quantum and another public and classic. If photons are the vehicle carrying the key, the quantum channel is usually an optical fiber. The public channel can also be so, but with one difference: in the quantum channel, there is in principle only one photon per bit to be transported, while in the public channel, in which eavesdropping by any non-authorized person does not matter, the intensity is hundreds of times bigger.

Step 1. Alice prepares photons with linear polarizations randomly chosen among the angles 0° , 45° , 90° and 135° , which she sends “in a row” through the quantum channel, while keeping a record of the sequence of the prepared states, as well as of the associated sequence of 0s and

1s obtained representing by 0 the choices of 0 and 45° degrees, and by 1 otherwise. This sequence of bits is clearly random. For instance, denoting by H, V, D and A the horizontal, vertical, 45° and 135° polarizations, respectively, and by +, \times the polarization basis $\{H, V\}$, $\{D, A\}$, possible Alice's sequences are:

```
++++x+xx+x++++xx+xx+xxx+x+++x+xxx+xxx+x++++x...
VVVHVAVAHVHDDVDDHHAHVHDHVVDVDAHVDAHVHVA...
11101111110100001000011110001101010101010100011...
```

Step 2. Bob has two analyzers, one “rectangular” (+ type), the other “diagonal” (\times type). Upon receiving each Alice's photon, he decides at random what analyzer to use, and writes down the aleatory sequence of analyzers used, as well as the result of each measurement. He also produces a bit sequence associating 0 to the cases when the measurement produces a 0° - or 45° -photon, and 1 in cases 90° and 135° . With the following analyzers chosen at random by Bob, a possible result of Bob's action on the previous Alice's sequence is

```
x+x+xxxx+++x+x+x+xxxx++++++xxxx+++x+xxxxxx+x+...
DVAHADAAVVDHDDHDAVDADAHVHVHVDADHVVDVAAADADHDDH...
01101011110000001101010010101001001101111010000...
```

Step 3. Next they communicate each other through the public channel the sequences of polarization basis and analyzers employed, as well as Bob's failures in detection, but never the specific states prepared by Alice in each basis nor the resulting states obtained by Bob upon measuring.

Alice to Bob: ++++x+xx+x++++xx+xx+xxx+x+++x+xxx...
 Bob to Alice: x+x+xxxx+++x+x+x+xxxx++++++xxxx++...

Step 4. They discard those cases in which Bob detects no photons, and also those cases in which the preparation basis used by Alice and the analyzer type used by Bob differ. After this distillation, both are left out with the same random subsequence of bits 0, 1, which they will adopt as the shared secret key:

```
Alice 11101111110100001000011110001101010101010...
++++x+xx+x++++xx+xx+xxx+x+++x+xxx+xxx+x...
Bob x+x+xxxx+++x+x+x+xxxx++++++xxxx+++x+xxxx...
011010111100000011010100101010010011011110...
```

```
Alice -1-01-111-0-000---0--1--10-01-0-0--10-1--0...
Bob -1-01-111-0-000---0--1--10-01-0-0--10-1--0...
```

Therefore the distilled key is 1011110000011001001010..., and its length is, on average, and assuming no detection failures, one half of the length of each initial sequence.

b. Eavesdropping effects.

All this holds in the ideal case that there are not eavesdroppers, neither noises in the transmission nor defects in the production, reception and analysis: the distilled keys of Alice and Bob coincide. But let us assume that Eve “taps” the quantum channel, and that, having the

same equipment as Bob's, analyzes the polarization state of each photon, forwarding them next to Bob. Ignoring Eve, much like Bob, the state of each photon sent by Alice, she will use the wrong analyzer with probability $1/2$, and will replace Alice's photon by another one, so that upon measurement Bob will get Alice's state only with probability $3/8$, instead of the probability $1/2$ in absence of eavesdropping. Therefore this intervention of Eve induces on each photon a probability of error $1/4$. Returning to the previous example, let us assume that Eve's measurements on Alice's photons produce the following results:

```
Eve x++x++++x++xxx+++++x+xxxx+xx+x+++x+xxx+x...
DVVAVVVVDVHADAVHVVHHHAAADHHDHDDVVDHAAADV...
```

These Eve's states are now those reaching Bob, who with his sequence of analyzers will obtain, for instance

```
x+x+xxxx++x++x+x+xxxx+++++xxxx++x+xxxxxx++x...
DVDVADADHVHAHHDHAHAHAHHAHHHHHDDDAVVAVADDDAAHHAH...
0101101001010000101111000000000111111000110010...
```

Proceeding as in step 4:

```
Alice 11101111110100001000011110001101010101010...
++++x+xx+x++++xx+xx+xxx++x+++x+xxx+xxx++x...
Bob x+x+xxxx++x++x+x+xxxx+++++xxxx++x+xxx...
0101101001010000101111000000000111111000...
```

```
Alice -1-01-111-0-000---0--1--10-01-0-0--10-1--0...
Bob -1-11-100-0-000---1--1--00-00-0-1--11-1--0...
```

We see that the coincidences in the distilled lists get disrupted: in 1 out of 4 cases, the coincidence disappears. Sacrificing for verification a piece of the lists taken at random from the final sequences, Alice and Bob can publicly compare them, and their differences will detect the intervention of Eve. If the length of that checking partial sequence is N , the probability that Eve's listening has not produced discrepancies is $(3/4)^N$, and thus negligible for N large enough. Therefore, should they not find any discordance, they can feel safe about the absence of eavesdroppers. But that binary string they have made public, they must clearly disregard it and not use it for coding. However, in practice both the emitting source, as well as the receiving equipment and the transmission channel display noise, which necessarily spoils, even with no snooping Eve, the perfect fit of the bit sequences distilled by Alice and Bob. It is necessary then to coexist with error, whenever this stays under a tolerable limit. In these circumstances, Eve will try to behave herself taking care that the effects of her listening stay below a certain threshold and do not shoot the alarm.

Cryptanalysts like Eve usually are quite more subtle in their perversity than what the previous simple analysis might suggest. Aware as they are of the quantum subtleties, they are not satisfied to incoherently tapping the quantum channel qubit to qubit; they are quite well knowledgeable that the coherent attack to strands of qubits, with probes analyzed after the public exchange of

information between Alice and Bob, can be much more rewarding. To prove the safeness of a protocol such as this BB84 under any type of imaginable attack by the malicious and cunning Eve is neither a trivial nor uninteresting issue, specially having in mind that other protocols resorting to quantum laws and considered as unconditionally secure have fallen down, as for example the *bit commitment* quantum protocol: Alice sends something to Bob under the firm commitment of having chosen a bit b that Bob completely ignores, but such that Alice can later show it to him when he claims it. Resorting to entangled EPR states makes it possible that any party of the couple behave dishonestly (that a cheating Alice change her commitment at the end without Bob being aware, or that a villain Bob gets some information on b without any request to Alice) (Mayers, 1996; 1997; Brassard et al., 1997).

There exists a proof of unconditional security of QKD through noisy channels and up to any distance, by means of a protocol based upon the sharing of EPR pairs and their purification, and under the hypothesis that both parties (Alice and Bob) have fault-tolerant quantum computers (Lo and Chau, 1999). Likewise, it is also claimed the unconditional security of the BB84 protocol (Mayers, 1998).

c. B92 Protocol.

Unlike the previous protocol, that uses a system in four states, pairwise orthogonal, in this somewhat simpler protocol B92 systems in only two non-orthogonal states are involved. Its analysis is similar to the previous one and shall be skipped.

3. EPR Protocols

In 1991 Ekert, relying on previous ideas of Deutsch, proposed an elegant method for secret key distribution, where the generalized Bell's inequality is on the watch to safeguard the confidentiality in the transmission of pairs of spin $\frac{1}{2}$ particles entangled *à la* EPRB (Deutsch, 1985; Ekert, 1991).

Six months after appearing Ekert's work, Bennett, Brassard and Mermin (1992) presented a very simple scheme for key distribution that keeps using EPRB states in the singlet state ($2^{-1/2}(|01\rangle - |10\rangle)$), but does not need to invoke Bell's theorem to detect Eve's listening. Alice and Bob measure the spin of their respective subsystems (halves of EPRB pairs) randomly along Ox or Oz . Through a public channel, they inform each other about their sequences of selected observables, but not of the results $\pm\frac{1}{2}$ obtained. They discard the cases in which their selections differ. They keep the remainder; the results of the latter are evidently anticorrelated. Bob reverses now all his outcomes ($\pm\frac{1}{2} \mapsto \mp\frac{1}{2}$), and then both Alice and Bob add $\frac{1}{2}$ to their results, thereby obtaining the secret

key to be shared. Sacrificing as before a piece of the key for its public comparison, they can detect Eve's listening.

Although it can be shown that this protocol is essentially equivalent to the BB84 (Bennett, Brassard and Mermin, 1992), it presents a potential bonus (Collins, 1992): the users (Alice and Bob) could wait for the key to show up just when they were about to use it (should they know how to keep the EPR states expectant for a while between their production and use), removing this way the possibility of robbery by Eve of the shared key.

C. Practical Implementation of QKD

The BB84 protocol was implemented by the first time in the IBM T.J. Watson Research Center (1989-1992) with polarized photons over 32 cm in air (Brassard, 1989; Bennett et al., 1992). In 1995 the B92 protocol was realized experimentally, also with polarized photons, transmitted this time through optical fibre 22.8 km long in the Swisscom cable connecting the cities of Geneva and Nyon under the Leman lake (Muller, Breguet and Gisin, 1993; Muller, Zbinden and Gisin, 1996).

The use of photon polarization states for long distances has a disadvantage: birefringency in the non-straight parts of the fiber transforms linearly polarized states into states of elliptic polarization, with accompanying losses in transmission, and further produces dispersion of the orthogonal polarization modes. Thereby the interest in other ways to codify the states, like for example by means of phases instead of polarizations. A group from the British Telecom from UK accomplished it (1994) with optical fiber over 30 km distance, using interferometry with phase-encoded photons (Marand and Townsend, 1995). There are no major difficulties in reaching around 50 km. In 1999 a group from Los Alamos has reached 48 km using this procedure (Hughes et al., 1996; 1999a; 1999b). For that reason it can be used to safely connect diverse agencies of the Government in Washington. To cover distances larger than 100 km would require the use of safe repeaters where key material for re-broadcasting might be generated.

With the protocol B92 again, it was possible in 1998 to quantumly transmit the secret key, at a rate of 5 kHz and over 0.5 km in broad daylight and free space, with polarized photons (Hughes et al., 1999a; 1999c). With this key Alice encrypted a photograph (with 8 bits per pixel), which Bob decrypted to reconstruct the primitive image, with the results shown in Fig. 7.

In the near future this procedure can be used to generate secret keys, shared by earth-satellite or satellite-satellite, that allow to protect the confidentiality of the transmissions.

More recently, QKD over 360 m has been achieved using variants of E91 and BB84 (Jennewein et al. 1999). They used pairs of entangled photons to generate keys at a rate 0.4-0.8 kHz with an error bit rate of about 3%.

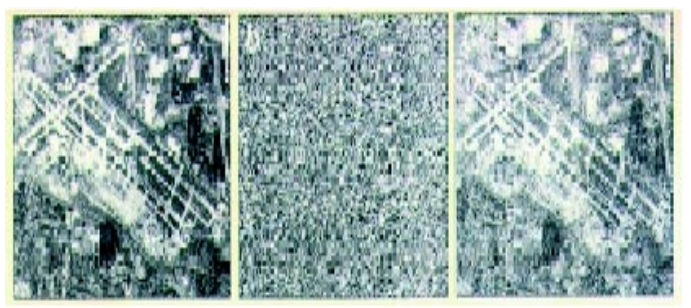


FIG. 7: Air view of St. Louis airport (left), encrypted image with a quantumly generated key (center), and decrypted image (right).

VII. QUANTUM COMPUTATION

A simple and intuitive way to arrive at the notion of quantum computation is through the *miniaturization*.²⁷ This has been the driving force in the modern upgrade of ordinary computers. As a matter of fact, the electronic industry of computers grows at the same time as the integrated circuits decrease in size. This rapid growth in the industry will continue as long as it is possible to include more and more circuits in a single chip. However, this pace cannot last forever and at some point it will reach the limits of the integrated circuits technology. Even if we can overcome these technological barriers, this trend will head us to the quantum realm where the quantum laws of physics will impose fundamental limitations on the size of the circuit components and on their performance. Thus, if the computer industry is to keep growing at the same rate, it will require another technological revolution.

Although this may look quite well ahead, it is estimated that about the year 2020 we shall reach the atomic size for storing one bit. Instead of just waiting for this situation to come, some theoretical physicists decided to move ahead and started to wonder about the radical changes and possible advantages that a computer may have if based upon the principles of the quantum mechanics.

The estimations for reaching the atomic scale are based in a remarkable observation made by Gordon Moore (1965), later known as *Moore's law*, that the number of transistors per square inch on integrated circuits had doubled every year since the integrated circuit was invented. Explicitly, the original curve for the density of silicon integrated circuits (transistors per square inch) was $\propto 2^{(t-1962)}$ where t is the calendar year. In subsequent years, the trend slowed down a bit, but chip capac-

²⁷The famous Feynmann's speech addressing the American Physical Society (1959), with his provocative bets on building micro-engines and writing on pin heads, signals the birth of *nanotechnology*.

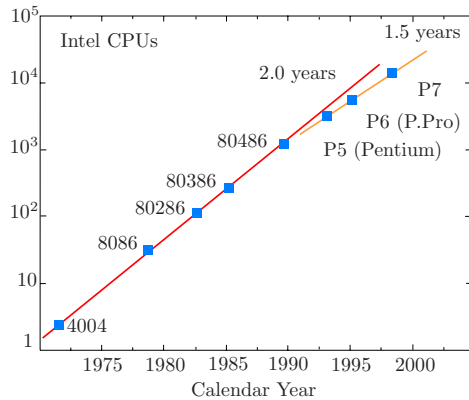


FIG. 8: Moore's law for processors capacity (number of transistors per square inch).

ity has doubled approximately every 18-24 months, and this is the current definition of Moore's law (see Fig. 8).

VIII. CLASSICAL COMPUTERS

To pave the way to the concept of quantum computers it proves convenient to discuss a classical concept, namely, the notion of *classical parallel computation*. To properly understand this let us recall first the basic principles operating most of the ordinary computers we work with as they were introduced first by Turing in 1936 and subsequently developed by Von Neumann in 1945 (Von Neumann, 1945; 1946), among others.

A. The Turing Machine

The concept of a *Turing Machine* (TM) has become the foundation of the modern theory of computation and computability: the study of what computers can and cannot do. Turing arrived at this concept in 1936 (Turing, 1936) in his quest to answer one of the questions posed by Hilbert. This was the *problem of decidability* (Entscheidungsproblem): Does it exist, at least in principle, a definite method or process by which all mathematical questions can be decided? (Hodges, 1992).

Turing realized that addressing this problem would require a precise and compelling definition of what a *definite method* is, as it appears in the statement of Hilbert's problem. This is what Turing achieved by analyzing what a person does during a methodically process of reasoning. His guiding idea was how to translate the human process of thought into something purely "mechanical", and then he went on to map that process into a "theoretical machine" which would operate on symbols on a paper tape according to precisely defined elementary rules. Turing also provided convincing arguments that the capabilities

of such a machine would be enough to encompass everything that would amount to a *definite method*, which in modern language is what we call an *algorithm*.

We shall see later how Turing answered the question of decidability in the negative using his concept of a TM, which we should first introduce.

A *Turing Machine* is a type of Finite State Machine (FSM) which has a finite set of states $\mathcal{S} = \{s_1, s_2, \dots, s_S; s_{S+1} = s_{\text{halt}}\}$, a finite alphabet of symbols $\mathcal{A} = \{a_1, a_2, \dots, a_A; a_{A+1} = \text{blank}\}$ and a finite set of instructions $\mathcal{I} = \{i_1, i_2, \dots, i_I\}$. In addition, it has an external infinitely long memory tape. This is called a (S -state, A -symbol) TM.

The states s_i correspond to the functioning modes of the machine and the TM is exactly in one of these states at any given time. The symbols in the alphabet serve to encode the information processed by the machine: they are used to code input/output data and to store the intermediate operations. The instructions are associated to the states in \mathcal{S} and they tell the machine what action to perform if it is currently scanning a certain symbol, and what state to go into after performing this action. There is a single *halt* state s_{halt} (or halt, for short) from which no instructions emerge, and this halt state is not counted in the total number of states. There is also a *blank* symbol which serves to separate strings of data coded with the rest of the alphabet symbols.

All these elements ($\mathcal{S}, \mathcal{A}, \mathcal{I}$) are physically arranged as follows. A TM consists of three components:

The *tape*, which is a doubly-infinite tape divided into distinct sections or cells. Each cell can hold only one symbol $a_i \in \mathcal{A}$.

A *Read/Write (R/W) head or cursor*, which can read or write the symbol $a_i \in \mathcal{A}$ in each tape cell.

A *control unit*, which is a device (or box) that controls the movements of the R/W head based on the current state of the TM and the content of the cell currently scanned by the R/W Head, i.e., based on a pair (s_i, a_i) .

The R/W head is capable of only three actions:

Write on the tape (or erase from tape), only the cell being scanned.

Change the internal state.

Move the head one cell to the left or right. Let us denote this variable as $\gamma \in \{L, R\}$.

The behaviour of a TM is governed by the set of instructions \mathcal{I} . These are rules which describe the transition from an initial pair (state, symbol) to a final pair plus the movement of the R/W head. Thus, each instruction $j \in \mathcal{I}$ is a 5-tuple $[(s_i, a_i), (s_f, a_f; \gamma)]$ representing the following transition

$$\mathcal{I} \ni j : (s_i, a_i) \mapsto (s_f, a_f; \gamma). \quad (54)$$

A consistency condition is demanded: no two instructions $j_1, j_2 \in \mathcal{I}$ have the same initial pair (s_i, a_i) .

In Fig. 9 we plot a schematic picture of a TM.

An alternative and efficient way to describe a TM is by means of a *flow* or *state diagram* (see Fig. 10). Here each

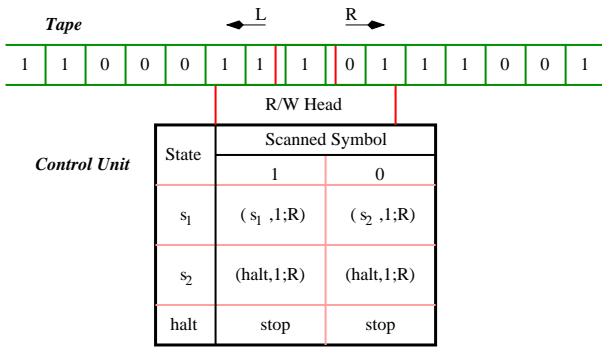


FIG. 9: A picture showing the components of a Turing Machine. The alphabet $\{1;0\}$ is unary, with 0 denoting blank. Stop means that $(s_{halt}, .)$ has no assigned instruction.

state $s_i \in \mathcal{S}$ is enclosed in a circle, and the instructions associated to a couple of states are represented by arrows showing also the change of symbols on the tape and the head movement.

In Fig. 10 we show a (2-state,1-symbol) TM. It is customary in this case to use a 1 for the symbol and 0 for the blank, i.e., $\mathcal{A} = \{1;0\}$. When $A = 1$ and $S = 2$ we talk of a 2-state TM for brevity. Then, this is a unary machine, which should not be confused with a binary system, since each number n is represented as a string of n 1s on the tape, and not by its binary representation. The state set is $\mathcal{S} = \{s_1, s_2; halt\}$. In this simple example of TM, when it is in state s_1 scanning a 1, the machine will move Right one cell and stay in state s_1 (this is the loop in Fig. 10). When it is in state s_1 scanning a blank symbol, it will change this symbol to a 1 and go to state s_2 . When it is in state s_2 , it will just move Right and stop.

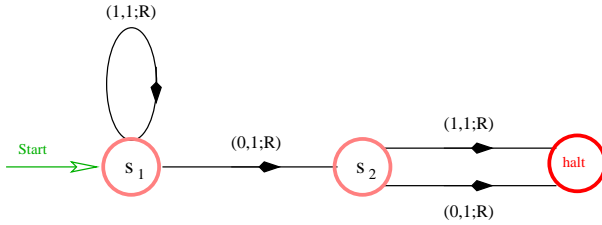


FIG. 10: An example of flow diagram for a (2-state,1-symbol) Turing Machine as shown in Fig. 9.

In summary, unless it is in the halt state, this simple TM will march rightward as long as it scans 1s, and when it meets its first blank symbol, it will change this into a 1 and then it will move Right twice and stop.

Let us now describe a TM performing a more interesting task like adding two numbers. This is a Adding TM. Suppose we want to sum $n_1 + n_2$. The input data in the tape is a string of n_1 1s separated by a 0 from another string of n_2 1s. The output data in the tape must be a string of $n_1 + n_2$ 1s. To achieve this output, we need

to remove the leftmost 1 in n_1 and convert the 0 into a 1. Then we can use a 2-state TM defined as follows (see Fig. 11). When it is in state s_1 and the R/W Head scans a 1, there is a transition to state s_2 , the 1 is replaced by 0 and the head moves to the right. Similarly, there are other 3 instructions which we plot in Fig. 11 in the form of a chart table of instructions. In this Fig. 11 the input is $2 + 2$ and the output 4.

1. Computability

Despite their simplicity, Turing machines can be devised to compute remarkably complicated functions. In fact, a TM can compute anything that the most powerful ordinary classical computer can compute. Until the formulation of Quantum Computing, none had yet proposed a model of computation more powerful than the TM. Thus, if we stick to classical machines and we had to solve problems which a TM cannot solve, it seems that we would have to resort to “supermachines” performing infinitely many steps in a finite time or to guess the answer out of the blue or something similar. The formalization of this idea into a proposition was done independently by A. Church and A. Turing and goes by the name of *Church-Turing hypothesis* (Church, 1936; Turing, 1936; 1950; Hodges, 1992). Following Turing, it is stated as: Every function that would naturally be regarded as computable can be computed by some Turing Machine.

This is a hypothesis because it cannot be proved unless we provide a formal definition of what *naturally* means. This hypothesis has not been refuted within the realm of classical physics, but we shall see that the notion of a Quantum Turing Machine requires to reformulate the Church-Turing thesis.

As a consequence of the Church-Turing hypothesis, a function is called *computable* when it can be computed by a TM, while it is declared a *noncomputable* function otherwise.

2. The Universal Turing Machine

A further crucial concept introduced by Turing is that of the Universal Turing Machine (UTM) (Turing, 1936). So far we have considered TMs built for a specific purpose and for that purpose only. The Universal TM allows us to run all TMs on a general machine. Thus, a UTM is defined as a single machine which comprises all Turing Machines and is therefore capable of computing any algorithm.

Just as an ordinary TM is defined by a set $(\mathcal{S}, \mathcal{A}, \mathcal{I})$ with the instructions in \mathcal{I} being described by a 5-tuple $[(s_i, a_i), (s_f, a_f; \gamma)]$, a UTM is constructed likewise by providing a set $(\mathcal{S}_U, \mathcal{A}_U, \mathcal{I}_U)$ and a description of its instructions $[(S_i, A_i), (S_f, A_f; \Gamma)]$. These instructions of a

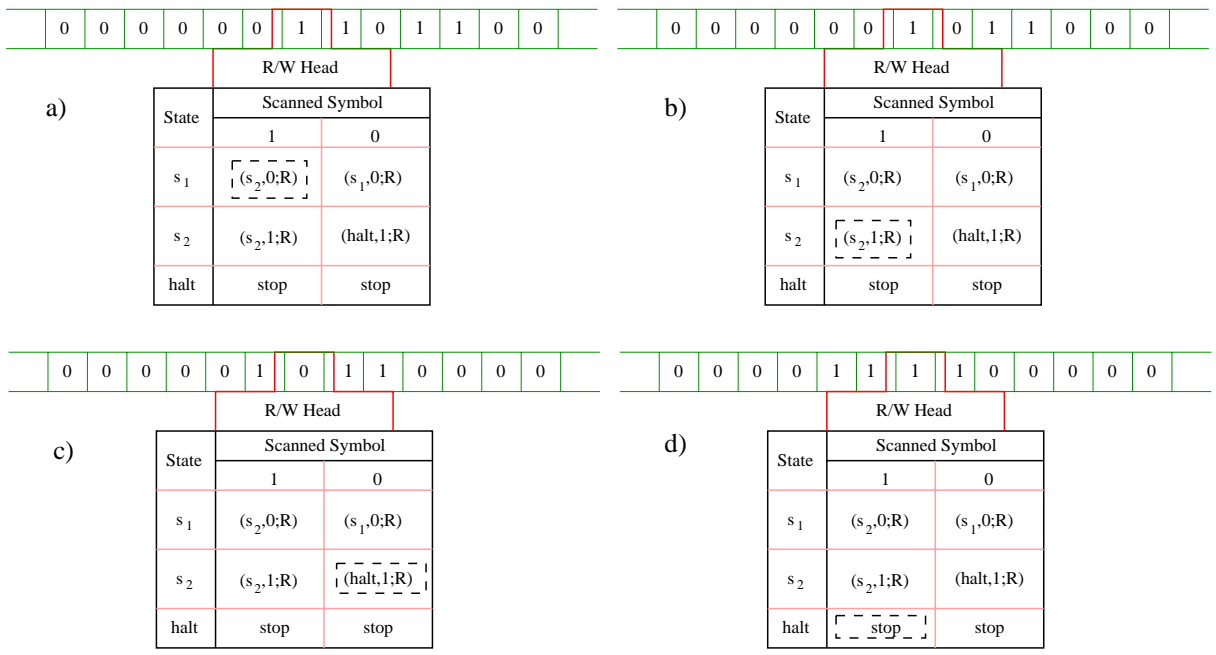


FIG. 11: An example of Adding Turing Machine: following the sequence of instructions in the Control Unit the machine performs $2 + 2 = 4$.

UTM must be general enough to accommodate any possible TM. This is accomplished by supplying it with the information of a TM and the data of its tape.

There are several ways to construct explicitly a UTM (Herken, 1995; Feynman, 1996; Minsky, 1967). For simplicity, let us assume that the alphabet $\mathcal{A}_U = \{a_1 = 0, a_2 = 1; \mathcal{A}'_U\}$ has a binary part corresponding to \mathcal{A} . This is not a restriction since any alphabet \mathcal{A} can be mapped onto a binary alphabet. At any given step of the functioning of a UTM, the initial pair (S_i, A_i) will know about the current description of the TM's tape, and as it also knows about the set of instructions \mathcal{I} , then the UTM will output exactly the same data as the TM it is simulating. In order to implement this, we need to accommodate quite a lot of, but finite, information in the UTM's tape. Namely, the input data for the UTM's tape is precisely all we need to know about the TM it reproduces: $(\tau; (\mathcal{S}, \mathcal{A}, \mathcal{I}))$, where τ denotes the TM's tape. These elements are disposed on the UTM's tape consecutively and separated by marks belonging to \mathcal{A}'_U . The R/W head of the UTM is positioned at the initial cell of the string encoding the data pair (s_0, a_0) of the TM. Then the UTM starts working, resorting to its set of instructions \mathcal{I}_U . Without going into further details, this set contains rules specifying how to bring the R/W head to read a pair (s_i, a_i) , change it to a new pair (s_f, a_f) and find the movement γ of the tape τ . This is repeated all over until the given TM is fully imitated.

The number of states S_U and symbols A_U is variable in a UTM. Minsky has constructed one with $S_U = 7$, $A_U = 4$ (Minsky, 1967). In fact, one can in principle construct

always a UTM with only $S_U = 2$ and finitely many symbols, or only $A_U = 2$ and finitely many states.

The importance of the universal machine is clear. We do not need to have an infinity of different machines doing different jobs. A single one will suffice. The engineering problem of producing various machines for various jobs is replaced by the office work of *programming* the universal machine to do these jobs (Turing, 1948). In summary, a TM is comparable to an algorithm much like the UTM is to a programmable computer.

3. Undecidability. The Halting Problem

With the aid of a TM, Turing was able to answer the problem of decidability. This can be rephrased in terms of TMs: is it possible to compute *any* function by designing an appropriate TM? Turing showed that this is not possible because the set of possible functions is much larger than the set of possible TMs. In fact, the set of TMs is denumerable (and so is the set of inputs). This is because any TM can be encoded into a finite binary string. However, it is possible to find sets of functions which are uncountable. Turing provided one such example due to Cantor: the set \mathcal{F} of all functions $f : \mathbb{N} \rightarrow \mathbb{N}$. Cantor had shown fifty years earlier, with his dilemma of diagonalization, that this set \mathcal{F} was not countable. The proof is simple, by reductio ad absurdum: assume \mathcal{F} is denumerable, then label each function $f \in \mathcal{F}$ with an integer: $\mathcal{F} = \{f_0, f_1, \dots, f_n \dots\}$. Next construct a function $g : \mathbb{N} \rightarrow \mathbb{N}$ by defining $g(k) := f_k(k) + 1, \forall k$. This function g is new, it is not contained in the initial set

\mathcal{F} since it differs for at least one value of the argument from each function in \mathcal{F} . Thus, the set \mathcal{F} is not complete. Contradiction.

This analysis implies that there must be noncomputable functions. Turing provided the first explicit example known as *the halting problem*: is it possible to design a TM H which tells us whether *any* TM will halt or not, when executing its procedure for *any* input? Turing showed that there does not exist such a TM H (Turing, 1936), in other words, the halting decision problem is undecidable, or equivalently, the predicate ($\{0,1\}$ -valued function) $h : \mathbb{N} \times \mathbb{N} \ni (i, j) \mapsto 1$ if the i -th TM T_i will halt for input j , $h : (i, j) \mapsto 0$ otherwise, is noncomputable.²⁸ In fact, suppose that the contrary holds, i.e. that there exists H which computes h , and define a function $\bar{h} : x \mapsto 1$ if $h(x, x) = 0$, $\bar{h}(x)$ being undefined otherwise.²⁹ The function \bar{h} is computable by a TM \bar{H} obtained from H just by replacing 0 by 1 when H halts and outputs 0, and by entering an endless loop when H is ready to halt with output 1. Let $\bar{H} = T_{i(\bar{H})}$; if $\bar{h}(i(\bar{H}), i(\bar{H})) = 1$, then $h(i(\bar{H}), i(\bar{H})) = 0$ and thus \bar{H} should not halt for input $i(\bar{H})$. Contradiction. Similarly, if $\bar{h}(i(\bar{H}), i(\bar{H}))$ is not defined, then $h(i(\bar{H}), i(\bar{H})) = 1$ and thus \bar{H} should halt for input $i(\bar{H})$. Contradiction again. Therefore H cannot exist.

Another example was provided by T. Rado (1962) with the so called Rado's Σ -function: assume that the TM has S states, $A = 1$ symbols and the input data is a tape completely blank. Then, $\Sigma(S)$ is defined as the maximum number of 1s left on the tape after this S -state TM halts. This type of TM is now known as *the busy-beaver problem*. Busy beavers TMs are difficult to find for two reasons (Shallit, 1998): firstly, the search space is extremely large – there are $[4(S+1)]^{2S}$ TMs with S states (for each non-halting state there are two transitions out, so the total of transitions is $2S$, and each transition has 2 possibilities for the symbol being written, 2 possibilities for the direction to move $\gamma = L, R$, and $S+1$ possibilities for what state to go to – including the halting state). Secondly, due to the halting problem, it is in general not possible to determine whether a particular TM will halt. We have to content ourselves with finding busy beavers for small S by a brute-force approach. In Table II we show the current status of this search. Another Rado's function $\Sigma'(S)$ appears which is the maximum number of moves performed by the TM before halting. Clearly, $\Sigma'(S) \geq \Sigma(S)$.

In Fig. 12 we plot an explicit flow diagram of a 3-state busy beaver (Shallit, 1998). When this TM starts with input data a completely blank tape, it executes 13 moves and writes six 1s. Thus, $\Sigma(3) \geq 6$ and $\Sigma'(3) \geq 13$. Lin

S	$\Sigma(S)$	$\Sigma'(S)$
1	1	1 ^a
2	4	6 ^a
3	6	21 ^a
4	13	107 ^b
5	≥ 4098	$\geq 47\,176\,870^c$

^a (Lin and Rado, 1965). ^b (Brady, 1983). ^c (Marxen and Buntrock, 1990).

TABLE II: This is a table of busy-beaver TMs for small S number of states. For $S = 6$, $\Sigma(6) \geq 95\,524\,079$, $\Sigma'(6) \geq 8\,690\,333\,381\,690\,951$ (Marxen, 1997).

and Rado showed (1965) that for $S = 3$ the $\Sigma(3)$ lower bound yields in fact the correct solution. From $S = 5$ on, only lower bounds are known. For example, $\Sigma(8) > 10^{44}$ (Rozenberg and Salomaa, 1994).

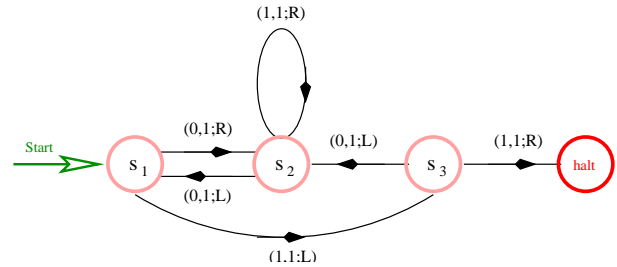


FIG. 12: A 3-state busy-beaver Turing Machine.

The proof that $\Sigma(S)$ is a noncomputable function goes by reductio ad absurdum. One shows that $\Sigma(S)$ grows with S faster than any computable function, i.e. if $F(S)$ is an arbitrary computable function, then there exists S_0 such that $\Sigma(S) > F(S)$ for $S \geq S_0$ (Shallit, 1998). As a byproduct, $\Sigma'(S)$ is not computable either.

4. Other Types of Turing Machines

The TMs considered so far are *deterministic*: the instructions $i \in \mathcal{I}$ follow the transition rules in (54). It is possible to design other TMs called *nondeterministic Turing machine* (NDTM) for which, given an initial pair (s_i, a_i) , there exists a bunch of possible final triplets (Yan, 2000). This means that the transition mapping (54) is no longer a function, but a *relation* given by

$$(\mathcal{S}, \mathcal{A}) \longrightarrow \text{Subsets}(\mathcal{S}, \mathcal{A}; \gamma) \quad (55)$$

where $\text{Subsets}(\mathcal{S}, \mathcal{A}; \gamma)$ denote all possible subsets of the Cartesian product $\mathcal{S} \times \mathcal{A} \times \gamma$. A *probabilistic Turing Machine* (PTM) is a type of nondeterministic Turing machine with some distinguished states called *coin-tossing states*. When the machine goes into one of these coin-tossing states, the control unit chooses between two possible legal next triplets in $\mathcal{S} \times \mathcal{A} \times \gamma$. The computation of

²⁸Any form of input/output can be encoded into nonnegative integers (Salomaa, 1989).

²⁹Note that the same integer x singles out here both a TM and an input.

a probabilistic TM is deterministic except that in coin-tossing states the machine tosses an unbiased coin to decide between two possible legal next moves. The class of NDTMs is more powerful than the class of deterministic Turing machines in the sense that anything computable with a TM is also computable with a NDTM and usually faster. A nondeterministic TM is closer to the idea of a Quantum Computer, but still it is far from one of them as we shall see in Sec. IX.

The Turing Machines introduced so far are *irreversible*: given the output of a computation we cannot generally reconstruct the input data. A *reversible* TM is one for which the input determines the output and conversely, the output determines the input. More explicitly, to each Turing machine M we can associate a directed configuration graph $\Gamma(M)$: each node of the graph is a possible configuration $C \in \mathcal{S} \times \mathcal{A}$, and two nodes C, C' are arc-connected when there is some instruction $i \in \mathcal{I}$ of M bringing C to C' in a single computation step.

Reversible Turing Machine: A Turing machine M is reversible iff its graph of configurations $\Gamma(M)$ has only nodes with indegree and outdegree³⁰ ≤ 1 .

We know that a non-reversible Turing machine has out-degrees ≤ 1 . It is apparent that demanding indegrees ≤ 1 implies that M can be executed in reverse deterministically, since every configuration has only one possible predecessor.

Lecerf (1963) and independently Bennett showed (1973) that an irreversible Turing machine can be simulated with a reversible Turing machine, at the expense of extra computer space and time. This is a remarkable fact for quantum computing since a quantum Turing machine must be reversible (see Sec. IX).

Not only Turing devised a theoretical computer, but he also pursued the practical construction of one of them. At the end of the war Turing was invited by the National Physical Laboratory (NPL) in London to design a computer. His report proposing the Automatic Computing Engine (ACE) was submitted in March 1946. Turing's design was at that point an original detailed design and prospectus for a computer in the modern sense. The size of storage he planned for the ACE was regarded by most who considered the report as hopelessly over-ambitious and there were delays in the project being approved. In the long run, the NPL design made no advance and other computer plans at Cambridge and Manchester took the lead. One year earlier von Neumann had pushed forward another project for constructing a computer machine.

B. The von Neumann Machine

The foundations of von Neumann's work on computers were laid down in the "First Draft of a Report on the EDVAC," written in the spring of 1945 and distributed to the staff of the Moore School of Engineering at the University of Pennsylvania (where the EDVAC was originally developed) in late June (Aspray, 1990). It presented the first written description of the *stored-program* concept and explained how a stored-program computer does process information. Von Neumann collaborated with Mauchly and Eckert on the design for EDVAC.

We can summarize the functioning of an ordinary computer by saying *one single thing at a time*. Von Neumann was the first to formalize the principles of a "program-registered calculator" based in the *sequential* execution of the programs registered in the memory of the computer. This is called a *von Neumann machine* (VNM). A VNM has the following parts which are depicted in Fig. 13:

Processor: The active part of the computer where the information contained in the programs is processed step by step. It is in turn divided into three main parts:

i) *Control Unit*: The unit which controls all the parts of the computer in order to carry out all the operations requested by other parts, such as extracting data from the memory, executing and interpreting instructions, etc.

ii) *Registers*: A very fast memory unit inside the processor which contains that part of the data which is currently being processed.

iii) *ALU*: The Arithmetic and Logic Unit which is devoted to the real computations such as sums, multiplications, logic operations, etc., executed on the data supplied by the registers or memory upon demand by the control unit.

Memory: The part of the computer devoted to the storage of the data and instructions to be processed. It is divided into individual cells which are accessible by means of a number called *address*.

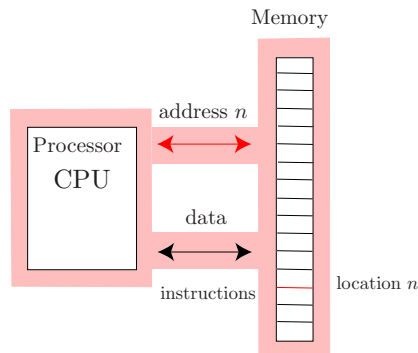


FIG. 13: Von Neumann Machine.

The functioning of a VNM is cyclic. One of these cycles contains the following operations: the control unit reads one program instruction from the memory, which

³⁰The indegree (outdegree) of a node is the number of incoming (outgoing) lines.

is executed after being decoded. Depending on the type of instruction, a piece of data can either be read from or written in the memory, or an instruction be executed. In the next cycle to be performed, the control unit reads another program instruction which is precisely next in the memory to the one processed in the previous cycle.

It is the simplicity of this sequentially operating model which makes it rather advantageous for many purposes because it facilitates the design of machines and programs.

C. Classical Parallelism

There are complex problems which demand a very large number of operations to be performed as well as a large amount of computer resources. These problems include image processing such as satellite images, meteorological predictions, scientific calculations arising in strongly correlated many-body systems, computation of the hadronic spectrum in QCD (Quantum Chromodynamics) on the lattice, real-time calculations in plasma physics, turbulence in fluids, and many more. It was noticed soon that an ordinary computer based on the VNM architecture would have a very long way to cope with such a type of problems where a massive number of operations is needed to be done in a very short period of time.

A classical parallel computer is the natural way to address these problems. The idea of parallelism is also simply summarized as *many things at a time*. We shall see that a quantum computer would realize this goal at the highest possible degree of parallelism.

Although the idea of parallelism is very simple to state, its practical implementation has faced many obstacles for several reasons we shall briefly describe. This will be quite illustrative later when we refer to the principles of quantum computation.

The way to extend the sequential VNM into a parallel computer is not unique. The components entering a parallel machine (PM) are already present in the VNM, but its number and organization differs. One way to understand the various possibilities is by recalling the organization of a program in any computer. A program is divided into *instructions* and *data*. These are its building blocks. This distinction means that we may have several degrees of parallelism depending on how many instructions and/or data the PM handles at a time. This leads to a first classification of PM's known as *Flynn's classification* (1966; 1972) which describes in four categories how a computer functions without entering the details of its architecture:

i) *SISD*: Single Instruction stream, Single Data stream. Executes one instruction at a time (single instruction stream) and fetches/stores one data value at a time (single data stream). It has only one CPU. Example: the von Neumann machine (specifically, processors like Motorola, Intel and AMD, etc.).

ii) *MISD*: Multiple Instruction stream, Single Data stream. This corresponds to multiple programs operating on the same data (performing different computations) Example: none is available. This category does not seem to be useful.

iii) *SIMD*: Single Instruction stream, Multiple Data stream. Executes one instruction at a time (single instruction stream) and the same operation is performed on many data values at the same time (multiple data stream). Example: The *vector machines* like Thinking Machine's Connection Machine CM-2. A vector operation with n elements can be executed by one instruction cycle on a SIMD parallel machine.

iv) *MIMD*: Multiple Instructions stream, Multiple Data stream. These are multiprocessor systems, each processor executing a different program on its own data. Thus, there are multiple instruction streams (programs) and multiple data streams. Example: most distributed memory parallel processors, like Thinking Machine's Connection Machine CM-5, Cray T3D, IBM SP-2, workstation clusters, fit in this category.

Of these machines, those of type SIMD and MIMD are parallel machines, the latter having a higher degree of parallelism. In Fig. 14 we show a schematic representation of Flynn's classification. Only processors and memory units are represented, without going into finer details about the interconnection network, types of memories (shared, distributed, cached, ...), pipelines, etc.³¹

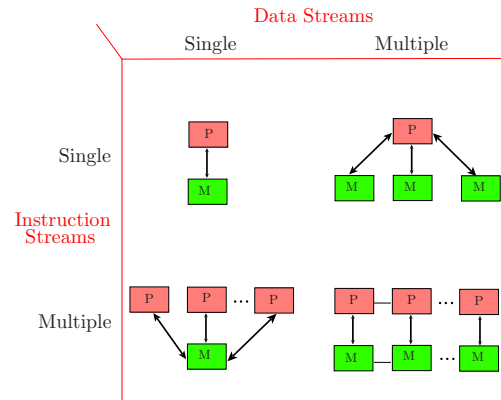


FIG. 14: Flynn's classification of parallel machines (P = processor, M = memory).

One may think at first glance that what counts in a PM is simply the number of processors. However, what really matters is the way the many processors are organized and how the information is exchanged among them. The reason is because for two processors to intercommu-

³¹ Flynn's classification is too coarse for classifying multiprocessor systems, and there exist modifications to it (Hwang and Briggs, 1985) and new ones as well like *Händler's classification* (1982) and others.

nicate, it is necessary that they be synchronized and consequently, they have to wait each other. Thus, this slows the functioning of a PM if only the number of processors is increased without taking care of their organization.

Therefore, we arrive at the conclusion that to scale up a PM one has to multiply the number of processors and to find out as well interconnecting structures for them. These structures or networks need be regular, efficient and low cost. The determination of the best interconnecting network for the processors in a PM is specially crucial when their number increases considerably.

For an interconnecting network (or lattice) to be good it has to minimize at the same time the total number of physical connections (or links) and the average distance between processors. This average distance is measured in terms of the number of connections to be traversed. Furthermore, the network has to be regular enough to allow being scalable when more processors are added.

In order to understand these requirements let us enumerate and analyze some archetypical networks.

Fully connected lattice: This is one extreme case which is made up of, say, N processors in such a way that all of them are connected one another, as shown in Fig. 15. The number of connections is $\frac{1}{2}N(N-1)$, and thus it is of order $O(N^2)$. This fact makes it non-practical because there are other more economical alternatives for connections.

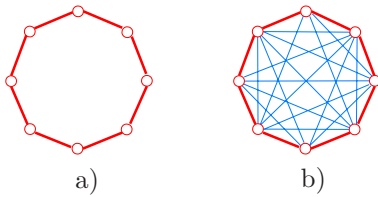


FIG. 15: Ring vs. fully connected processor lattices.

Ring lattice: The network of processors forms a ring (see Fig. 15), which has the advantage of needing only two connections per processors, no matter their number. In this sense it is opposite of the full lattice. However, it has a very important disadvantage, because in the worst case a message has to traverse $N/2$ processors (half of the lattice) to reach its destiny. This is also non-practical when N is large.

Binary Tree: The processors are organized such that each node is connected to three nodes, namely, one *parent* and two *children* (Fig. 16). The problem with this type of lattice is that the inner nodes deep inside the tree are very badly communicated among themselves.

Hypercube: This is the solution that has turned to be optimal in meeting the desired requirements (Fig. 17). In the simplest possibility, one processor is installed at each vertex of the cube, which can be of any dimension D . In the familiar case of a $D = 3$ cube, each processor is connected to other 3 and more importantly, each one is at a maximum distance of 3 connections from any other.

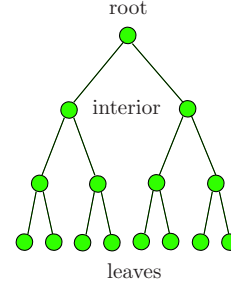


FIG. 16: Binary tree processor lattice.

For a D -dimensional hypercube the number of processors is 2^D , each one is connected to D neighbor processors and is at most a distance D apart from any other. The most famous PM based on this hypercube architecture is the original Connection Machine and the Crays. It is not surprising that Feynman, who played a paramount role in the beginning of quantum computers, worked in the design of this PM and made some notorious contributions (Hillis, 1998).

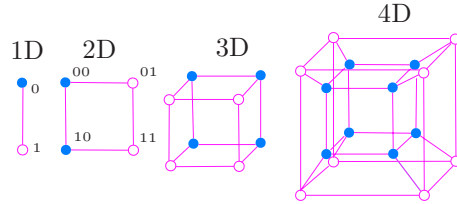


FIG. 17: Hypercube networks.

The interconnecting networks of processors considered so far are called *static* because the structure is fixed by construction. There exists also the possibility of *dynamic* networks where its configuration is changeable. In this case the processors are connected not directly but through commutators which can be switched in different ways.

One of the fundamental problems posed by the parallel computers is its control. There are also several strategies to address this issue. One possibility is to have a central processor working as a control unit for the rest of processors, as in the SIMD. This is a model of centralized control in which the control unit sends instructions to the other processors which never interfere the central processor. In order to simplify their working, it is normal that the same instruction is sent to all the processors which in turn operate on different sets of data. This mode of control has the same disadvantages as the original VNM: it is slow. The reason is because the control unit has to send many electrical pulses to perform the control task.

An alternative to centralized control consists in allowing each processor to take its own decisions, usually consulting only its nearest-neighbor processors. This solution has also difficulties because the programs must be

written in a way very different from the standard. Moreover, such non-centralized control can become very inefficient because the processors might spend most of their time exchanging messages rather than making computations.

The problem of organizing and controlling the parallelism in a classical computer resembles very much the organization problems in the human societies, which is as open a problem there as for networks of computers. We shall see in Sec. IX that in a quantum computer one also faces similar synchronization problems and we shall discuss how they are solved in terms of physical principles.

D. Classical Logic Gates and Circuits

A Turing machine is by no means a practical computer, despite of being a powerful theoretical machine. In practice, computers are made of electronic circuits, which in turn contain *logic gates*. A logic gate is a device that implements a classical *logic operator* like the AND operator. A logic operator or function f is an application $f : \{0, 1\}^n \mapsto \{0, 1\}^m$, which maps an input of n bit-valued operands into a m -bit-valued output. When the target space of f is $\{0, 1\}$, one usually says that f is a *Boolean operator* or function. A *Boolean algebra* is a unital algebra defined over the field $\mathbb{Z}_2 = \{0, 1\}$. Boolean algebras are useful to elucidate situations which can be true or false, making appropriate reasonings to draw conclusions correctly. They are therefore helpful in building practical computers and in programming. Furthermore, it is possible to show that classical Turing machines are equivalent to classical logic circuits. This means that they both have the same complexity classes. This is a mathematical result that legitimates the use of electronic circuits in the construction of real computers.

Before stating this important result as a theorem, let us take a closer look at some rudiments of Boolean logic that will also help in understanding the peculiarities of quantum logic gates (see Sec. IX).

An operator with one operand is called a *unary* operator, with two operands is a *binary* operator. There are three basic Boolean or logic operators: 1/ The unary operator NOT: $x \mapsto \text{NOT } x := \bar{x} := 1 - x$, denoted also by overlining the argument ($\bar{}$). 2/ The binary operator AND: $(x, y) \mapsto x \text{ AND } y := x \wedge y := xy$, also denoted by \wedge . 3/ And the binary operator OR, $(x, y) \mapsto x \text{ OR } y := x \vee y := x + y - xy$, denoted also by \vee . As usual, Boolean arithmetics is done in the field \mathbb{Z}_2 : $1 + 1 = 0$.

The action of a logic operator is represented by a *truth table*. A truth table contains as many columns as input operands and output bits, and $2^{\#\text{operands}}$ rows. The inputs are shown on the left, and the output is shown on the right. The truth tables for the basic operators are shown in Table III. An important Boolean expression involving 2 variables x, y is $r = (\bar{x} \wedge y) \vee (x \wedge \bar{y})$, i.e.

x	\bar{x}	x	y	$x \wedge y$	$x \vee y$
0	1	0	0	0	0
1	0	0	1	0	1
		1	0	0	1
		1	1	1	1

TABLE III: Truth tables for the basic logic operators: NOT ($\bar{}$), AND (\wedge), OR (\vee).

$r(x, y) = x + y$.³² Expressions in the Boolean algebra can be represented by *logic circuits*. A logic circuit is a directed acyclic graph with incoming lines carrying input Boolean variables x_1, x_2, \dots, x_n and an outgoing line carrying the output variable y of the circuit. Every node in the graph is a *logic gate* which represents a logic operator of the Boolean algebra. In real computers, circuits consist of electronic devices such as switches and wires.

To each logic operator we can associate a logic gate with a specific form. That logic gate has a number of incoming lines, one per input operand, and one outgoing line for the output result. In Fig. 18 we show the convention for the basic logic gates. In the same way as the basic operators of the algebra make up more complicated expressions, the basic gates are combined to construct complex circuits.

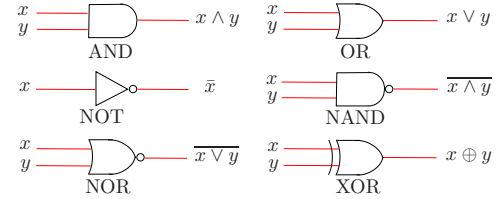


FIG. 18: Basic classical logic gates.

Additional gates that duplicate the input values on wires are frequently needed. These are called FANOUT or COPY gates and they are schematically represented by $\rightarrow \bullet <$ (see Fig. 19). In classical computation, these are sort of obvious gates for they simply correspond to splitting the wire into two or more leads, which is an easy operation. This is why they are usually taken for granted throughout classical computing. Nevertheless, these irreversible FANOUT gates are logically necessary when discussing the important issue of universality of classical gates. On the contrary, these duplicating gates find no room in the insides of a quantum circuit due to the linearity of quantum mechanics (no-cloning theorem, Sec. III).

A Boolean circuit computes a Boolean function in a natural way by following its directed path (usually from

³²This r corresponds to the XOR operation.

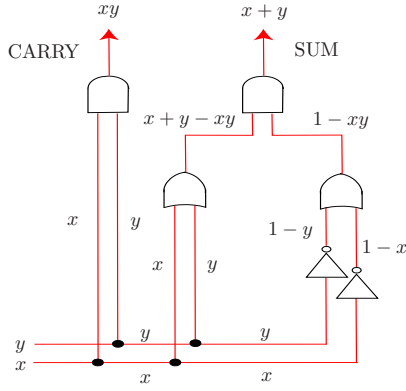


FIG. 19: A classical logic circuit: adder for two bits x, y . The bifurcating wires at the nodes are achieved with FANOUT gates.

left to right) upon application of its constituent gates. The *size* of a circuit C is its number of gates, and the *depth* of C is the length of the longest directed path in it. A typical circuit is depicted in Fig. 19.

Suppose that we are given a tractable decision problem, i.e. a problem in class \mathbf{P} (see Appendix). This means that there exists a Turing machine M deciding it ($M(x_n) = 0, 1$) for initial data x_n of arbitrary length n , in polynomial time. This problem is said to have *polynomial circuits* when there is a family $\{C_1, \dots, C_n, \dots\}$ of logic circuits, of polynomial size in the input length n , such that $M(x_n) = 0, 1$ iff $C_n(x_n) = 0, 1$.

It can be shown that all problems in class \mathbf{P} have polynomial circuits. The converse, however, is not true: there exist undecidable decision problems that have polynomial circuits (Papadimitriou, 1994). This shortcoming is remedied by restricting the circuit family to be a *uniform* circuit family: for each n , the description of each C_n is an output of an auxiliary Turing machine in polynomial time when entered with an appropriate input of length n .³³

The equivalence between classical Turing machines and Boolean logic circuits is stated in the following theorem (Savage, 1972; Schnorr, 1976; Pippenger and Fisher, 1979; Papadimitriou, 1994):

Turing machines and uniform circuit families: A decision problem is in class \mathbf{P} , i.e. it can be solved for inputs of length n by a Turing machine in polynomial time $p(n)$, iff it has a uniform family of polynomial circuits. Moreover, the minimum size of C_n is $O(p(n) \log p(n))$.

This theorem legitimates the simulation of Turing machines by logic circuits. Dealing with gates and circuits is simpler and more practical than with Turing machines. Actually, gates are packaged into hardware chips.

³³Actually the auxiliary TM should be $(\log n)$ -space bounded, what implies polynomial time boundedness.

So far we have introduced a set of three basic logic operators (NOT, AND, OR). It proves also convenient to introduce three additional new gates: NAND, NOR and XOR. The gates NAND and NOR are the negation of AND and OR, respectively. The gate XOR is called *exclusive* OR, and is also denoted by \oplus . Their truth tables are shown in Table IV.

x	y	x NAND y	x NOR y	x XOR y
0	0	1	1	0
0	1	1	0	1
1	0	1	0	1
1	1	0	0	0

TABLE IV: Truth tables for the logic operators NAND, NOR, XOR.

With the basic set $\{\text{NOT}, \text{AND}, \text{OR}\}$ one can build any logic function over the Boolean algebra, provided that FANOUT gates and ancilla or work bits are freely used. Because of this property, $\{\text{NOT}, \text{AND}, \text{OR}\}$ is called a *universal* set of logic gates. However, this set is not minimal. To see this we use the so called de Morgan's laws, which are the following Boolean identities:

$$\begin{aligned} \overline{(x \vee y)} &= \bar{x} \wedge \bar{y}, \\ \overline{(x \wedge y)} &= \bar{x} \vee \bar{y}. \end{aligned} \quad (56)$$

These two algebraic equations are dual each other. Negation of the first produces $x \vee y = \overline{(\bar{x} \wedge \bar{y})}$. This is telling us is that OR gates are not essential: the AND and NOT gates can by themselves reproduce the functionality of the OR gate. Similarly, the second relation in (56) leads to $(x \wedge y) = \overline{(\bar{x} \vee \bar{y})}$, that is, AND gates can be implemented with OR and NOT gates. Then the set $\{\text{AND}, \text{NOT}\}$ is universal, and so is the set $\{\text{OR}, \text{NOT}\}$.

Can we reduce further the number of elements in a universal set? The answer is yes. The surprising result is that NAND gates alone (or, similarly, NOR gates alone) are sufficient for constructing any circuit (up to FANOUT and work bits). We know this from the following simple laws:

$$\begin{aligned} \bar{x} &= 1 \text{ NAND } x, \\ x \wedge y &= \overline{(x \text{ NAND } y)} = 1 \text{ NAND } (x \text{ NAND } y). \end{aligned} \quad (57)$$

Therefore we see that $\{\text{NAND}\}$ (or $\{\text{NOR}\}$) can do everything that the set $\{\text{AND}, \text{NOT}\}$ does, and hence $\{\text{NAND}\}$, $\{\text{NOR}\}$ are also universal sets.

IX. PRINCIPLES OF QUANTUM COMPUTATION

In the previous section we have described some basic aspects of Turing machines and their practical implementations by means of the Von Neumann architecture. Yet, there is a long way from there towards the construction of

a real computer as those we have on our desks. In Fig. 20 we provide a visualization of the route we have to follow. This long route starts with the abstract notion of a classical computer embodied in a Turing machine. No real computer has a Turing machine inside. Instead, the operations carried out by a Turing machine can be substituted by *logic gates*. These logic gates can do sums, multiplications, logic operations, etc. With just a few logic gates we can do almost nothing of the daily tasks we are used to nowadays. To get the power and speed of an ordinary computer we need millions of logic gates interconnected and integrated into tiny circuits. These are called *integrated circuits* or *chips*. Finally, these integrated circuits are arranged into the computer motherboard with other components, and along with a screen, keyboard, mouse, etc. we have a universal machine capable of doing many tasks, like writing this article.

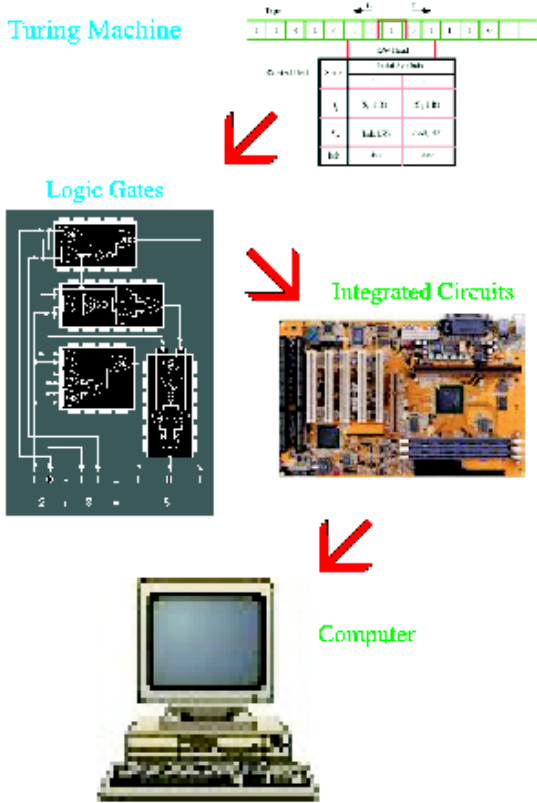


FIG. 20: From a Turing machine to a real computer.

All these four stages in Fig. 20 have been accomplished in the case of the classical computers. What is the current state of the art in the case of quantum computers? The first step in Fig. 20 has also been achieved for quantum computers. This is the topic of Subsec. IX.A where we discuss the notion of quantum Turing machines, the quantum version of the classical Turing machines introduced thus far. Moreover, the second step regarding the

design of quantum logic gates has also been accomplished as we shall explain in Subsec. IX.B. These quantum gates are used as the basic components of a quantum computer to design quantum algorithms that surpass certain very important classical algorithms (see Sec. X). More important is the fact that, in the recent years, an experimental realization of these quantum gates have been made (see Sec. XI), which let us cherish the possibility of building a real operative quantum computer on equal footing as the current classical precursors. However, to achieve this goal we need to move more steps farther like finding the quantum equivalent of an integrated circuit (third step). This step amounts to the problem of scalability in a quantum computer: so far, the experimental realization mentioned previously are made of a just a few gates and although a quantum gate is more powerful than a classical one, we also need a large number of them to make non-trivial tasks. We need to scale up our current quantum technology. Finally, the last fourth step will be to have a real operative quantum computer in our hands, with all the external devices to communicate with it. Although there is still a long way ahead to achieve this goal, the fact that the fundamental first and second steps have been already done is very encouraging. In the following we shall describe these two steps for quantum computers.

From a fundamental point of view, a quantum computer (QC) is a quantum Turing machine (QTM) and this is a concept that we shall next define.

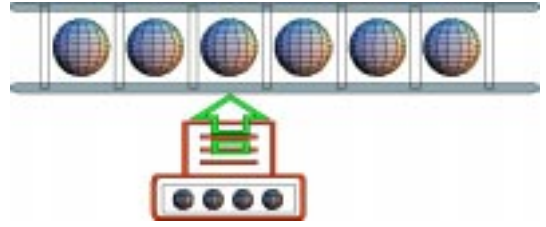


FIG. 21: Pictorial view of a quantum Turing machine: there are qubits (Bloch's spheres, Fig. 2) in the tape and in the control unit.

A. The Quantum Turing Machine

There have been several achievements before arriving at the concept of a QTM and it is not our purpose to give a full account of all of them, but instead we shall mention some of the most representative constructions or *machines*. We start mentioning the *Benioff's machine*, which is a model for computation introduced by P. Benioff (1980; 1981; 1982). Benioff's goal was to use quantum mechanical systems to construct reversible Turing Machines. His motivation was that the unitary evolution of an isolated quantum system provides a way to implement reversible computations. The issue of reversibility had attracted much attention since Bennett (1973) constructed a classical model of reversible computing ma-

chine equivalent to a Turing machine. Landauer (1961) had shown that reversible operations dissipate no energy, while a Turing machine as described in Sec. VIII performs irreversible changes during computations. Although the Benioff's machine is a quantum machine, it is not however a quantum computer for it is equivalent to a reversible TM. Feynmann (1982) went one step further towards the notion of quantum computer with his "universal quantum simulator" or *Feynman's machine*. He proposed to use quantum systems to simulate quantum mechanics more efficiently than classical computers do.³⁴ He showed (Feynmann, 1985) that classical TMs exponentially slow down when simulating quantum phenomena while a universal quantum simulator would do efficiently the job. However, Feynman's machine is not fully a quantum computer in the sense described below for it does not let program an arbitrary task.

Deutsch (1985) gave the final step in the quest of a sensible definition of a quantum computer. His starting point is a critique of the Church-Turing hypothesis (see Sec. VIII.A) which he considers very vague as compared to physical principles such as the gravitational equivalence principle. Deutsch's proposes to make more concrete the statement "functions which would naturally be regarded as computable" in Church-Turing hypothesis. He identifies such functions as those which can be computed by a real physical system. This is quite apparent, since it is hard to believe that something be naturally computable if it cannot be computed in Nature. Thus, Deutsch goes on to promote the Church-Turing hypothesis into a physical principle which he states as the *Church-Turing Principle*: Every finitely realizable physical system can be perfectly simulated by a universal model computing machine operating by finite means.

The content of this principle is more physical than the corresponding hypothesis since it appeals to objective concepts such as measurement, physical system, etc. instead of the subjective notion of "naturally computable". The "finite means machine" in the Church-Turing principle is more general and replaces the role of the Turing machines in the corresponding hypothesis (Sec. VIII.A).

Deutsch follows a natural way to introduce the definition of a *Quantum Turing Machine* (QTM): starting from the knowledge we have of its classical counterpart (see Sec. VIII.A) he replaces some of the classical components of an ordinary TM, like bits, by quantum elements, like qubits.

A *Quantum Turing Machine* is a Finite State Machine which has three components: a *finite processor*, an infinite *memory unit* (of which only a finite portion is ever used) and a cursor. The description of these components is as follows:

- i) *Finite Processor*: This is the control unit as in a

TM but it consists of a finite number P of qubits. Let us denote the Hilbert space of these processor states as

$$\mathcal{H}_P := \text{span}\{\otimes_i |p_i\rangle : p_i = 0, 1\}_{i=0}^{P-1}. \quad (58)$$

- ii) *Memory Tape*: This has a similar functionality as in a TM but it consists of an infinite number of qubits.³⁵ Let us denote the Hilbert space of these memory states as

$$\mathcal{H}_M := \text{span}\{\otimes_i |m_i\rangle : m_i = 0, 1\}_{i=-\infty}^{+\infty}. \quad (59)$$

- iii) *Cursor*: This is the interacting component between the control unit and the memory tape. Its position is scanned by a variable $x \in \mathcal{H}_C = \mathbb{Z}$, and the associated Hilbert space is

$$\mathcal{H}_C := \text{span}\{|x\rangle : x \in \mathbb{Z}\}. \quad (60)$$

Therefore, there is a Hilbert space of states associated to a QTM which altogether takes the form

$$\mathcal{H}_{QC} := \mathcal{H}_C \otimes \mathcal{H}_P \otimes \mathcal{H}_M. \quad (61)$$

The basis vectors in the Hilbert space \mathcal{H}_{QC} of the QTM are of the form

$$|x; \mathbf{p}; \mathbf{m}\rangle := |x; p_0, p_1, \dots, p_P; \dots, m_{-1}, m_0, m_1, \dots\rangle, \quad (62)$$

and are called the *computational basis states*.

We may wonder about the relationship between the defining features of a classical TM (see Sec. VIII.A) and those of a QTM. The set of states \mathcal{S} corresponds to the Hilbert space of states \mathcal{H}_P in a QTM. The alphabet \mathcal{A} is just the qubit space \mathbb{C}^2 . As for the set of instructions \mathcal{I} of a TM, we need to specify the way a QTM works.

A QTM operates in steps of fixed duration T , and during each step only the processor and a finite part of the memory unit interact via the cursor. We stress that a QTM, much like a TM, is a mathematical construction; we shall present explicit experimental realizations in Sec. XI.

The set of instructions \mathcal{I} of a TM is replaced by the unitary time evolution of the quantum states $|\Psi\rangle \in \mathcal{H}_{QC}$. After a number $n \in \mathbb{N}$ of computational steps, the state of the QTM will be transformed into

$$|\Psi(nT)\rangle = U^n |\Psi(0)\rangle, \quad (63)$$

with U a unitary evolution operator, $UU^\dagger = U^\dagger U = 1$. A valid quantum program takes a finite number of steps n . To each QTM there is associated a unitary evolution operator U to make a certain job or program, much like a TM has a unique set of instructions \mathcal{I} , and each TM makes a certain task. To specify the initial state $|\Psi(0)\rangle$,

³⁴Manin (1980) had already envisaged that the complexity of quantum systems surpassed the capabilities of classical computers.

³⁵Even if ideally there is a qubit per cell, only a finite number of them are active during each running of the QTM.

we set to zero both the cursor position $x = 0$ and the prepared processor states $\mathbf{p} = \mathbf{0}$. The memory states \mathbf{m} are prepared allocating the *input data* and other program instructions, conveniently encoded into a finite number of qubit strings, with the rest of the memory qubits set to $|0\rangle$. The initial state is then

$$|\Psi(0)\rangle = \sum_{\mathbf{m}} c_{\mathbf{m}} |0; \mathbf{0}; \mathbf{m}\rangle, \text{ with } \sum_{\mathbf{m}} |c_{\mathbf{m}}|^2 = 1. \quad (64)$$

The notion of a QTM operating “by finite means” entering the Church-Turing principle means that the machine cannot do infinitely many operations at a given time nor at arbitrary positions along the memory tape. This notion suggests the following constraint on the matrix elements of the evolution operator of a QTM:

$$\begin{aligned} \langle x'; \mathbf{p}'; \mathbf{m}' | U | x; \mathbf{p}; \mathbf{m} \rangle &= [\delta_{x', x+1} U^+(\mathbf{p}', m'_{x'} | \mathbf{p}, m_x) \\ &+ \delta_{x', x-1} U^-(\mathbf{p}', m'_{x'} | \mathbf{p}, m_x)] \prod_{x' \neq x \pm 1} \delta_{m_{x'}, m_x}. \end{aligned} \quad (65)$$

In these matrix elements, the infinite product guarantees that only a finite number of memory qubits participate in a single computational step. Once the qubit at the x th cursor position is singled out, the two deltas appearing in the brackets guarantee that the cursor position cannot change by more than one unit, either backward, forward or both. This operating mode amounts to locality in the tape space. We call the parts $U^\pm(\mathbf{p}', m'_{x \pm 1} | \mathbf{p}, m_x)$ of U forward and backward matrices at x , respectively. They represent the operators $P_{x \pm 1} U P_x$ in the computational basis, where P_x is the projection onto the Hilbert subspace of \mathcal{H}_{QC} consisting of the states with the cursor at the x th position. Unitarity of U is equivalent to $U^{\pm \dagger} U^\mp = 0$, $U^{+ \dagger} U^+ + U^{- \dagger} U^- = 1$. Each unitary operator $U\{U^-, U^+\}$ defines a QTM.

As with any other computer, we need a mechanism to cause the QTM to halt when the computation ends. In a quantum machine there is a severe constraint to do this because the principles of quantum mechanics do not allow us to observe or measure the QTM until it terminates. To know when this happens, we may set aside one of the qubits of the processor to signal the end. Let us choose the first qubit $|q_0\rangle$ to acquire the value 1 when the computation is over while it is 0 during the operations. The program does not interact with $|q_0\rangle$ until when it has reached the end. Thus, the state $|q_0\rangle$ can be monitored periodically from the outside without affecting the operation of a QTM.

So far we have set up several connections between the components of quantum and classical Turing machines. Moreover, to complete this comparison, we can also think about the relationships concerning their functioning. Does a quantum TM extend somehow the notion of a classical TM? Yes, and this relation turns out to be very physical and it will sound familiar to us. Firstly, not all classical TMs are closely related to a quantum TM, only those reversible classical TM will be, as follows from

the discussion above. Then, it is possible for a quantum TM to reproduce the functioning of a reversible classical TM (Deutsch, 1985) if we choose its unitary evolution operator to have the following form:

$$\begin{aligned} U^\pm(\mathbf{p}', m'_{x \pm 1} | \mathbf{p}, m_x) &= \\ \delta_{\mathbf{p}', \mathbf{A}(\mathbf{p}, m_x)} \delta_{m'_{x \pm 1}, B(\mathbf{p}, m_x)} \frac{1}{2} [1 \pm C(\mathbf{p}, m_x)] \end{aligned} \quad (66)$$

where \mathbf{A}, B, C are maps of $\mathbb{Z}_2^P \times \prod_{-\infty}^{+\infty} \mathbb{Z}_2$ into $\mathbb{Z}_2^P, \mathbb{Z}_2$ and $\{-1, 1\}$, respectively.

This form of dynamics guarantees that this particular QTM will remain in a computational basis state (62) at the end of each time step. This is precisely the way a classical TM operates. The requirement of reversibility is guaranteed by demanding that the mapping $(\mathbf{p}, m) \mapsto (\mathbf{A}(\mathbf{p}, m), B(\mathbf{p}, m), C(\mathbf{p}, m))$ be bijective.

Therefore, there is a particular limiting case in which a quantum TM becomes a reversible classical TM. This fact is somewhat reminiscent of the familiar *correspondence principle* of quantum mechanics to recover classical mechanics. This principle played a fundamental role in the development of the old quantum theory and the beginnings of the modern quantum mechanics. Here we are following a similar path by starting with a revision of the classical fundamentals of information and computation to thereby develop their quantum versions.

1. Quantum Parallelism

The capability of a quantum TM of being in several computational basis states at the same time is called *quantum parallelism*, and is one of the defining features of a QTM. The classical counterpart of this is the notion of classical parallelism introduced in Sec. VIII.C. The quantum version of doing “many things at a time” in a classical parallel computer is the possibility of being in *many states at a time* in a quantum computer. Furthermore, in a classical computer it is not enough to have a large number of processors connected in parallel in order to perform computations efficiently. It is also necessary to have all of them appropriately synchronized to avoid message jams and disruptive functioning of the several processors which would not operate coherently. Likewise, quantum parallelism is not enough to achieve a successful quantum computation. Recall that the result of a quantum computation is probabilistic. There is not a 100% certainty that after measuring the final output state it will contain the correct result we are searching for. We need to repeat the measurement several times in order to retrieve the correct value of the function or procedure for which the computer was devised. If we program the quantum computer carelessly, this number of measurements would be exponentially large, and all the potential advantages of quantum parallelism spoiled. What do we need to make good quantum programs? We need to reduce the number of trials to just a few. This fact will depend on how the evolution operator $U\{U^+, U^-\}$

and the initial memory states $|\mathbf{m}\rangle$ are prepared. In order to become good quantum programmers we must be smart enough so as to devise them in such a way that the maxima of the probability distribution in the output state correspond to the desired result, while the rest of possible results, which are useless for the purpose of our computation, must be somehow damped. We recognize this pattern of behaviour for the unitary operator $U\{U^+, U^-\}$ as the phenomenon of *constructive interference* of amplitudes in quantum mechanics. The typical example is the two-slit experiment.

We shall present explicit examples of how quantum parallelism and constructive interference work together when we deal with quantum algorithms in Sec. X. Now, we summarize these correspondences between classical parallel and quantum computers as follows:

Classical Parallel Computers

- i) many things at a time
- ii) synchronization of many processors



Quantum Computer

- i) many states at a time
- ii) constructive interference of many states

The quantum version of parallelism exceeds the classical one, for whereas in a quantum computer it is possible to have an exponentially large number of available states within a reduced space, this capacity seems unreachable in any known classical parallel computer.

In quantum mechanics there are some basic principles, like the correspondence principle, Heisenberg's principle, Pauli's principle, etc., which encode the fundamentals of that theory. The knowledge of those principles provide us with the essential understanding of quantum mechanics at a glance, without going into the complete formalism of that subject. A similar thing happens with other areas in physics. In computer science there are also guiding rules to devise the architecture of a computer (hardware) and the programs to be run (software). Likewise, in quantum computing we have seen that there are basic principles that serve us as a guide to get the most profit from a quantum computer. These principles refer to the ideas of quantum parallelism and quantum programming. We know that information and computation is physics. Thus, there must be a connection between the principles of quantum computation and the principles of quantum physics. It is useful to synthesize those relationships between both fields in the form of basic principles, as shown explicitly in Table V.

By principles of quantum computation we mean those rules which are specific to the act of computing according to the laws of quantum mechanics. In this table we indicate that the quantum version of parallelism is realized through the superposition principle of quantum

TABLE V: Principles of Quantum Computation.

<i>Computer Science</i>	<i>Quantum Physics</i>
1 st Quantum Parallelism	= Superposition Principle
2 nd Quantum Programming	= Constructive Interference

mechanical amplitudes; likewise the act of quantum programming a quantum computer should be closely related to constructive interference of those amplitudes involved in the superposition of quantum states in the registers of a quantum computer. We shall see these principles in action when studying quantum algorithms (see Sec. X) that supersede their classical counterparts. This fact expresses that the capabilities of a quantum Turing machine go well beyond those of a classical Turing machine. The superposition principle when applied to multipartite quantum systems like those of a quantum register (see eq. (71) below) yields the notion of entanglement (Sec. III.A, Sec. III.E).

2. Universal QTM

The notion of universal Turing machine can also be extended to quantum Turing machines. A standard QTM is capable of performing only the job for which it has been set up. This is so because the unitary operator $U\{U^+, U^-\}$ and the memory quantum states $|\mathbf{m}\rangle$ are chosen to do one specific task. Deutsch (1985) has shown that the elements $U\{U^+, U^-\}$ and $|\mathbf{m}\rangle$ of a QTM can be devised to simulate with arbitrary precision any other quantum computer. This is the concept of *universal quantum Turing machine*. A universal QTM is thus a programmable quantum computer. We now give more explicit details about how a quantum TM is programmed.

Let f be the any function that we want to compute with the universal QTM, and let $\pi(f)$ be a quantum program to do the job. The quantum computer will take the program $\pi(f)$ and a given input value i and then compute the desired value $f(i)$. This process is implemented in a QTM as follows. There exists an integer n_{fin} such that

$$U^{n_{\text{fin}}} |0; \mathbf{0}; \pi(f), i, \mathbf{0}\rangle = |0; 1, \mathbf{0}; \pi(f), i, f(i), \mathbf{0}\rangle, \quad (67)$$

where the halting qubit is set to $|1\rangle$ after the computation ends. In this expression we assume that the initial quantum memory states are

$$|\mathbf{m}_{\text{in}}\rangle = |\pi(f), i, \mathbf{0}\rangle, \quad (68)$$

while the final memory states contain the answer $f(i)$:

$$|\mathbf{m}_{\text{fin}}\rangle = |\pi(f), i, f(i), \mathbf{0}\rangle. \quad (69)$$

If in eq.(67) we focus only on the memory states, then we can use a short-hand notation for the unitary evolu-

tion,³⁶ namely,

$$|\pi(f), i, j\rangle \mapsto |\pi(f), i, j \oplus f(i)\rangle. \quad (70)$$

Although a QTM has an infinite-dimensional memory space, much like a classical TM, we remark that only a finite-dimensional unitary transformation needs be applied at every step of the computation to simulate the associated QTM evolution.

The concept of a quantum Turing machine has many implications that we shall continue to present. Most of these implications amount to a revision of the typical areas of classical computation in the light of the new principles of computation. For instance, now we can immediately address how the theory of complexity gets affected in its fundamentals. In Sec. VIII.A we mentioned that this theory deals with the issue of what a computer can do. Namely, it studies not only which function can be computed, but also how fast and how much memory resources are needed. This scheme must be modified to convert it into a *quantum complexity theory*. In this new theory of complexity we must pose another question, “with which probability” can a quantum computer achieve a certain task. See Appendix for details.

B. Quantum Logic Gates

The quantum Turing machine is a basic model for quantum computation that deals with the new characteristics posed by quantum principles at a fundamental level, as compared with the classical functioning of a classical Turing machine. However, a quantum TM is not a practical starting point for designing a quantum computer, much like the classical Turing machine is not a handy computer.

The key idea is to decompose the functioning of a quantum computer into the simplest possible primitive operations or gates. The identification of universal logic gates, such as NAND, in classical computers (see Sec. VIII.D) was of great help in the development of the field. A universal gate such as NAND operates locally on a very reduced number of bits, actually two. However, combining NAND gates in the appropriate number and sequence we can carry out arbitrary computations on arbitrarily many bits. This was very useful in practice for it allowed device engineers to just focus on creating only a few devices, leaving the rest to the circuit designer. The same rationale applies to a quantum computer and the relation of a quantum Turing machine to quantum circuits.

When a quantum computer is working, it is an evolution unitary operator that is effecting a predetermined action on a series of qubits. These qubits form the memory register of the machine or a *quantum register*. A

quantum register is a string of qubits with a predetermined finite length. The space of all the possible register states makes up the Hilbert space of states associated to the quantum computer. If \mathcal{H} is the Hilbert space of a single qubit and $|\Psi_i\rangle \in \mathcal{H}$, $i = 1, 2$, a given basis state, then a basis vector $|\Phi\rangle$ for the states of the quantum register is a tensor product of qubit states

$$|\Phi\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle \otimes \dots \otimes |\Psi_n\rangle \in \mathcal{H}^{\otimes n}. \quad (71)$$

A quantum memory register can store multiple sequences of classical bits in superposition. This is a manifestation of the quantum parallelism.

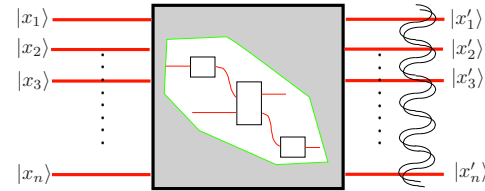


FIG. 22: A generic quantum logic gate. The wavy lines mean that the output state is a generic superposition of product quantum states.

A *quantum logic gate* is a unitary operator acting on the states of a certain set of qubits. If the number of such qubits is n , the quantum gate is represented by a $2^n \times 2^n$ matrix in the unitary group $U(2^n)$. It is thus a *reversible* gate: we can reverse backwards the action, thereby recovering the initial quantum state from the final one. Generically, a quantum logic gate can have any finite number of input qubits, but in practice we shall be interested in gates that are elementary for quantum computation, and those have a small number of input qubits. Diagrammatically, a quantum gate is represented by a “black box” wherein operation takes place, and a number of input (output) lines, used to wire up a set of gates, equal to the number of qubits involved in the computation (see Fig. 22). Let us see more explicitly how quantum gates look like by giving some representative gates in increasing order of complexity.

1-Qubit Gates. These are the simplest possible gates for they take one input qubit and transform it into one output qubit. The *quantum NOT* gate is a one-qubit gate. Its unitary evolution operator U_{NOT} is (11):

$$U_{\text{NOT}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (72)$$

The truth table and the diagram representing this gate are shown in Table III and Fig. 23, respectively. We see that this quantum NOT gate coincides with its classical counterpart. However, there is a basic underlying difference: the quantum gate acts on qubits while the classical gate does it on bits. This difference allows us to intro-

³⁶See Sec. IX.C for more on quantum function evaluation.

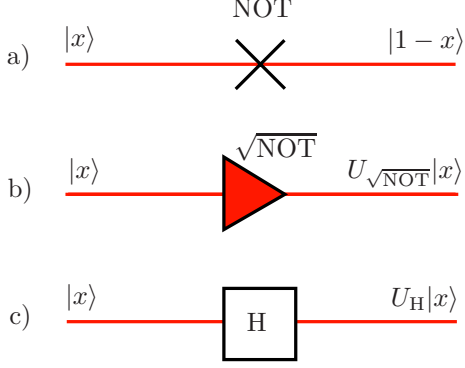


FIG. 23: Quantum unary gates: a) NOT gate, b) $\sqrt{\text{NOT}}$ gate, c) Hadamard gate.

duce a truly quantum one-qubit gate: the $\sqrt{\text{NOT}}$ gate.³⁷ Its matrix representation is

$$U_{\sqrt{\text{NOT}}} := \frac{1}{\sqrt{2}} e^{i\pi/4} (1 - i\sigma_x). \quad (73)$$

This gate, when applied twice, gives NOT. Explicitly

$$\begin{aligned} U_{\sqrt{\text{NOT}}} U_{\sqrt{\text{NOT}}} &= \begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix} \cdot \begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = U_{\text{NOT}} \end{aligned} \quad (74)$$

This gate has no counterpart in classical computers since it implements nontrivial superpositions of basis states.

Another one-qubit gate without analogue in classical circuitry and heavily used in quantum computations is the so called Hadamard gate H (see Sec. III). It is defined as

$$U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (75)$$

2-Qubit Gates. The XOR (*exclusive-OR*), or CNOT (*controlled-NOT*) gate, is an example of a quantum logic gate on two qubits (12). It is instructive to give the unitary action $U_{\text{XOR}, \text{CNOT}}$ of this gate in several forms. Its action on the two-qubit basis states is

$$\begin{aligned} U_{\text{CNOT}}|00\rangle &= |00\rangle, & U_{\text{CNOT}}|10\rangle &= |11\rangle, \\ U_{\text{CNOT}}|01\rangle &= |01\rangle, & U_{\text{CNOT}}|11\rangle &= |10\rangle. \end{aligned} \quad (76)$$

From this definition we see that the name of this gate is quite apparent for it means that it executes a NOT operation on the second qubit conditioned to have the first qubit in the state $|1\rangle$. Its matrix representation is

$$U_{\text{CNOT}} = U_{\text{XOR}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \quad (77)$$

The action of the CNOT operator (76) immediately translates into a corresponding truth table as in Table VI. The diagrammatic representation of the CNOT gate is shown in figure 24.

x	y	x'	y'
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

TABLE VI: The truth table of the quantum CNOT gate.

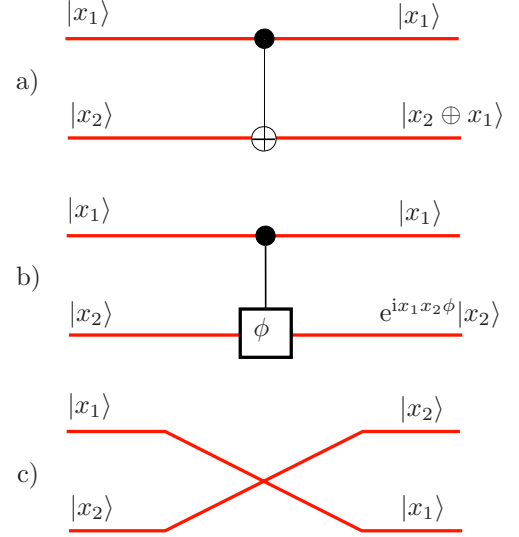


FIG. 24: Quantum binary gates: a) CNOT gate, b) CPHASE gate, c) SWAP gate.

We shall see how this quantum CNOT gate plays a paramount role in both the theory and experimental realization of quantum computers. It allows implementing conditional logic at a quantum level.

Unlike the CNOT gate, there are two-qubit gates with no analogue classical gate. One example is the *controlled-phase* gate or CPHASE:

$$U_{\text{CPh}(\phi)} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix} \quad (78)$$

It implements a conditional phase-shift $e^{i\phi}$ on the second qubit.

An important result is that we can reproduce the CNOT gate with a controlled-phase gate of $\phi = \pi$ and two Hadamards transforms on the target qubits as shown in Fig. 25. This is a simply consequence of the relation

$$U_H \sigma_z U_H = \sigma_x. \quad (79)$$

³⁷ Square-root-of-NOT gate.

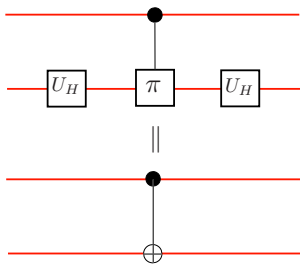


FIG. 25: Relation between CNOT gate and controlled-phase using Hadamard gates.

x	y	z	x'	y'	z'
0	0	0	0	0	0
0	0	1	0	0	1
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
1	0	1	1	0	1
1	1	0	1	1	1
1	1	1	1	1	0

TABLE VII: Truth table for the Toffoli gate.

Other interesting two-qubit gates are the SWAP gate, which interchanges the states of the two qubits, and the $\sqrt{\text{SWAP}}$ gate,³⁸ whose matrix representations are

$$U_{\text{SWAP}} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad U_{\sqrt{\text{SWAP}}} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1+i}{2} & \frac{1-i}{2} & 0 \\ 0 & \frac{1-i}{2} & \frac{1+i}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (80)$$

3-Qubit Gates. An immediate extension of the CNOT construction to three-qubits yields the CCNOT gate (or C^2NOT),³⁹ which is also called Toffoli gate T (Toffoli, 1981). The matrix representation is a one-qubit extension of the CNOT gate, namely

$$U_{\text{CCNOT}} = U_{\text{T}} := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (81)$$

The associated truth table is shown in Table VII. The first two input qubits x, y are copied to the first two out-

put qubits x', y' (see Fig. 26), while the third output qubit z' is the XOR of the third input z and the AND of the first two inputs x, y .

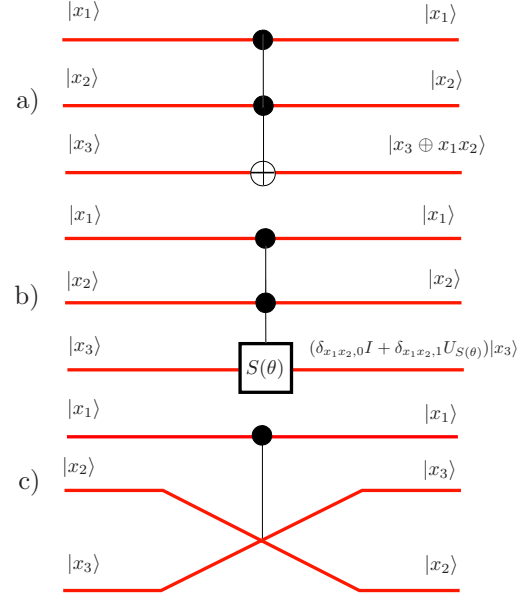


FIG. 26: A set of three-qubit gates: a) Toffoli gate, b) Deutsch gate, c) Fredkin gate.

The Deutsch gate $D(\theta)$ (Deutsch, 1989) is also an important three-qubit gate. It is a *controlled-controlled- S* or C^2S operation (see Fig. 26), where

$$U_{S(\theta)} := ie^{-i\frac{1}{2}\theta\sigma_x} = i\cos\frac{1}{2}\theta + \sigma_x\sin\frac{1}{2}\theta \quad (82)$$

is a unitary operation that rotates a qubit about the x axis by an angle θ and then multiplies it by a factor i . We demand θ to be *incommensurate* to π , that is, not a rational multiple of π . Several properties follow: 1) Let $|q\rangle$ be a given qubit, then for any fixed value of $\alpha \in \mathbb{R}$ we can get arbitrarily close to $e^{i\alpha\sigma_x}|q\rangle$ by successive application of $U_{S(\theta)}$ to $|q\rangle$ a finite number of times. 2) The Deutsch gate generates as closely as needed the Toffoli gate. This is because the C^2S^n gate is just the D^n gate. And since we can make $\frac{1}{4}(n\theta/\pi - 1)$, with $n = 4k + 1$, as near to a given arbitrary integer as desired, D^n will thereby approach closely the Toffoli gate.

Another instance of a three-qubit gate is the Fredkin gate F (Fredkin and Toffoli, 1982). It is a *controlled-SWAP* operation, schematically shown in Fig. 26 and represented by the matrix

$$U_{\text{F}} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (83)$$

³⁸Square-root-of-swap gate.

³⁹Controlled-controlled-not gate.

Needless to say that these unitary linear gates not only act on the basis states, but also on any linear combination of them.

We have enumerated a series of quantum logic gates whose use and importance will be explained in the following sections. We shall address the experimental implementation of some of these quantum gates in Sec. XI.

C. Quantum Circuits

The simple gates introduced in the previous section can be assembled into a network-like arrangement that enable us to perform more complicated quantum operations than those initially carried out by those gates. This is the basic idea of a *quantum circuit*. Deutsch (1989) generalized the classical reversible circuit model to produce the idea of quantum circuits. A quantum circuit is a computational network composed of interconnected elementary quantum gates.

An example to illustrate a simple use of a quantum circuit is the following. Let us prepare initially a one-qubit state as an arbitrary superposition of the logical states $|0\rangle, |1\rangle$, namely

$$|\psi_0\rangle = a|0\rangle + b|1\rangle. \quad (84)$$

We want to obtain a final state of GHZ type (22):

$$|\psi_f\rangle = a|000\rangle + b|111\rangle. \quad (85)$$

To this purpose, instead of writing a pertinent sequence of algebraic operations, we can simply arrange the following quantum circuit using the CNOT-gate as pictured in Fig. 27.

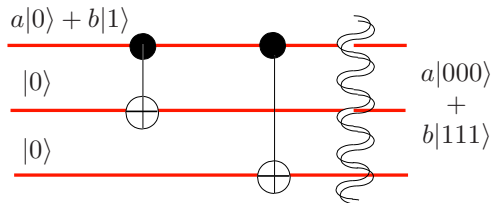


FIG. 27: An example of quantum circuit implementing a GHZ state.

Quantum circuits are widely used in quantum computation, where most of the problems can be formulated in terms of them. Moreover, it might quite well be the case that standard quantum mechanics could be flooded with quantum circuits in the future, something similar to what happened with Feynman diagrams in quantum field theory. The reason is because quantum circuits are able to condensate graphically much more information than the use of several formulas. Besides, this form of presenting and reasoning about is closer to what experimental physicists really do with their devices.

In Sec. VIII.D we presented the basic result that a classic Turing machine is equivalent to a classical logic

circuit. In quantum computing there is a similar result due to Yao (1993) showing that a quantum Turing machine is equivalent to a quantum circuit. This theorem justifies replacing the more complicated study of quantum Turing machines by that of quantum circuits, which are simpler to analyze and design. In fact, experimental approaches to quantum computers are presented in terms of quantum circuits (see Sec. XI).

Let K be a quantum Boolean or logic circuit with n input qubits. Suppose that $|\Psi_x\rangle = \sum_{y \in \{0,1\}^n} c_x(y)|y\rangle$ is the final quantum state of K for an input $x \in \{0,1\}^n$. The *distribution generated* by K for the input x is defined as the map $p_x : y \in \{0,1\}^n \mapsto |c_x(y)|^2$. The quantum circuit K is said to (n, t) -simulate a quantum Turing machine Q if the family of probability distributions p_x , $x \in \{0,1\}^n$, coincides with the probability distributions of the Q configurations after t steps with input x .⁴⁰ Then Yao's theorem is the following statement:

Quantum Turing machines and quantum circuits: Let Q be a quantum Turing machine and n, t positive integers. There exists a quantum Boolean circuit K of polynomial size in n, t , that (n, t) -simulates Q .

This result implies that quantum circuits can mimic quantum Turing machines in polynomial time, and vice versa. Thus, quantum circuits provide a sufficient model for quantum computation that is easier to implement and manipulate than QTMs. This situation goes in parallel with similar results about classical Boolean circuits and Turing machines (Sec. VIII.D). From now on when talking about a quantum computer we shall usually refer to an underlying equivalent quantum circuit.

1. Universal quantum gates

After the works of Deutsch (1989) and Yao (1993) the concept of a *universal set* of quantum gates became central in the theory of quantum computation. A set $\mathcal{G} := \{G_{1,n_1}, \dots, G_{r,n_r}\}$ of quantum gates G_{j,n_j} acting on n_j qubits, $j = 1, \dots, r$, is called universal if *any* unitary action U_N on N input quantum states can be decomposed into a product of successive actions of G_{j,n_j} on different subsets of the input qubits. More explicitly, given any U_N acting unitarily on N qubits, there exists a sequence S_1, S_2, \dots, S_s of subsets of $\{1, 2, \dots, N\}$, with n_{S_1}, \dots, n_{S_s} elements, and a map $\pi : \{1, 2, \dots, s\} \rightarrow \{1, 2, \dots, r\}$ such that $n_{\pi(j)} = n_{S_j}$, $\forall j$, and

$$U_N = U_{N, G_{\pi(s)}, S_s} \dots U_{N, G_{\pi(1)}, S_1}. \quad (86)$$

Here

$$U_{N, G_{\pi(j)}, S_j} := I_{\{1, 2, \dots, N\} - S_j} \otimes U_{G_{\pi(j)}, S_j}, \quad (87)$$

⁴⁰We assume that a given configuration is encoded as a list of the tape symbols from cell $-t$ to t , followed by the state and the position of the cursor, all encoded as strings of qubits (see Sec. IX.A).

where $I_{\{1,2,\dots,N\}-S_j}$ is the identity on the qubits not in S_j , and $U_{G_{\pi(j),S_j}}$ stands for the unitary action of the gate $G_{\pi(j)}$ on the Hilbert space of the n_{S_j} qubits in the set S_j .

For instance, a generic unitary $k \times k$ matrix of dimension $k \geq 2$ can be represented as the product of $k(k-1)/2$ two-level unitary matrices (Reck et al., 1994).

This notion of universal set of gates is *exact* for the generic transformation U_N is reproduced exactly in terms of a finite number of elements in \mathcal{G} . We denote this situation by writing the universal set as \mathcal{G}_{ex} . However, this notion is too strong. Dealing with practical quantum devices, it is not conceivable to work with a set of gates implementing any other gate with perfect accuracy. Thus, we are inevitably led to work with approximate simulations of gates. Underlying this idea there is the concept of distance between two unitary gates.

A quantum gate U_N is said to be approximated by another gate U'_N with error $< \epsilon$, when the distance $d(U_N, U'_N) := \inf_{\theta \in \mathbb{R}} \|U_N - e^{i\theta} U'_N\|$ between both matrices as projective operators is $< \epsilon$.^{41,42} This means that if the gate U_N is replaced by gate U'_N in a quantum circuit K , then the unit rays of the associated output states will differ in norm by at most ϵ .⁴³

With this definition, we also introduce the notion of an *approximate* set of universal quantum gates as before but with the weaker requirement that it simulates any other quantum gate in an approximate sense. We denote these sets as \mathcal{G}_{ap} , and by universality we shall mean it in this sense henceforth, unless the exact notion is explicitly indicated.

Some examples of universal sets of quantum gates, to be discussed next, are the following (for a more mathematical and general approach, see Brilynski et al., 2001):

1. $\mathcal{G}_{\text{ex}}^{\text{I}} := \{U_2 : U_2 \in \text{U}(2^2)\}$, (DiVincenzo, 1995).
2. $\mathcal{G}_{\text{ex}}^{\text{II}} := \{U_1, \text{CNOT} : U_1 \in \text{U}(2)\}$, (Barenco et al., 1995).
3. $\mathcal{G}_{\text{ap}}^{\text{III}} := \{\text{D}\}$, Deutsch gate (82), (Deutsch, 1989).
4. $\mathcal{G}_{\text{ap}}^{\text{IV}} := \{\text{C}^2\text{-}U, \text{C}^2\text{-}W\}$, with $U(\alpha) := R_y(4\pi\alpha) = e^{-i2\pi\alpha\sigma_y}$, $W(\alpha) := \text{diag}(1, e^{i2\pi\alpha})$, α an irrational root of a degree-2 polynomial (Aharonov, 1998).
5. $\mathcal{G}_{\text{ap}}^{\text{V}} := \{\text{H}, \text{CPh}(\frac{\pi}{2})\}$, (75), (78), (Solovay, 1995; Kitaev, 1997; Cleve, 1999).

6. $\mathcal{G}_{\text{ap}}^{\text{VI}} := \{\text{H}, W, \text{CNOT}\}$, with $W := \text{diag}(1, e^{i\pi/4})$, (Cleve, 1999).

Of these examples, 1/ and 2/ correspond to *infinite* sets of universal gates. However, a practical quantum computer must have a set with a *finite* number of universal gates. Examples 3/ to 6/ are finite suitable cases. Although with a finite set of gates we are limited to simulate a countable subset of all possible quantum gates, it is possible to reproduce an arbitrary gate within a given small error ϵ . Moreover, a finite universal set \mathcal{G}_{ap} is closer to the spirit of the Church-Turing principle stating that a computing machine must operate by finite means (Sec. IX.A).

A first example of 3-qubit universal gate is the Deutsch gate (Deutsch, 1989),⁴⁴ which is an extension of the Toffoli gate U_{CCNOT} (81) (Toffoli, 1981) for classical Boolean circuits. Toffoli gates are exactly universal for reversible (classical) circuits.⁴⁵ Deutsch showed that his gate $\text{D}(\theta_0)$ with a fixed angle θ_0 that is an irrational multiple of π is universal.

A further improvement in the analysis of quantum universal gates was provided by DiVincenzo (1995) who showed that the set of two-qubit gates is exactly universal for quantum computation. This is a remarkable result since it is known that its classical analogue is not true: classical reversible two-bit gates are not sufficient for classical computation. The NAND gate, although binary, is not reversible.

After DiVincenzo's result it was shown that a large subclass of two-qubit gates are universal (Barenco, 1995) and moreover, that almost any two-qubit gate is universal.

The reduction from three to two qubits amounts to a big simplification in the analysis of quantum circuits and in their experimental implementation. It is much simpler to deal with two-body quantum interactions than with a three-body problem.

The race towards bringing down the number of necessary qubits in the elementary gates culminated with the joint work of Barenco et al. (1995) in which it is shown that even one-qubit gates are enough for quantum computation (in the exact sense) provided they are combined with the CNOT gate. This result, another manifestation of the superposition principle, is quite surprising since in classical computation the classical CNOT is not universal.

⁴¹The norm $\|A\|$ of the (finite) matrix A is usually defined as $\sup_{x: \|x\|=1} \|Ax\|$. Other norms are topologically equivalent to it.

⁴²A compactness argument shows that the inf in the definition of d is attainable, i.e. $\exists \theta_0$ such that $d(U_N, U'_N) := \|U_N - e^{i\theta_0} U'_N\|$. From now on, we will assume that the phase factor is included in the approximating unitary operator U'_N .

⁴³The unit ray of a state vector $|\phi\rangle$ is the set $[\phi] := \{e^{i\theta}|\phi\rangle : \theta \in \mathbb{R}\}$. A distance between unit rays can be defined as $\text{dist}([\phi_1], [\phi_2]) = \inf_{\theta \in \mathbb{R}} \|\phi_1 - e^{i\theta}\phi_2\|$, what justifies the presence of a phase factor in the notion of an approximate gate.

⁴⁴Previously Deutsch (1985) had already given a universal set of eight 2×2 matrices.

⁴⁵To see that $\text{C}^2\text{-NOT}$ is classically universal, notice that: $1/ \text{NOT}(x_3) = (\text{CCNOT}(1, 1, x_3))_3$; $2/ \text{AND}(x_1, x_2) = (\text{CCNOT}(x_1, x_2, 0))_3$; and apply now the result (Sec. VIII.D) that $\{\text{AND}, \text{NOT}\}$ is a classical universal set. See in addition that the COPY operation is also reproduced as $\text{COPY}(x_2) = (\text{CCNOT}(1, x_2, 0))_{2,3}$.

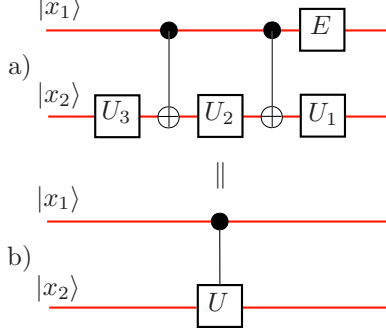


FIG. 28: Decomposition of an arbitrary two-qubit CU gate into one-qubit gates and CNOTs. The symbol E denotes the gate $E : |0\rangle \mapsto |0\rangle, |1\rangle \mapsto e^{i\delta}|1\rangle$.

We shall refer to this important result as the *universality theorem of elementary quantum gates*. The proof of this result (Barenco et al., 1995) can be simply stated in terms of quantum circuits and it has three parts. Firstly, we need to prove that with one-qubit gates plus CNOT it is possible to generate any controlled-unitary two-qubit gate. Secondly, this result is extended to a controlled-unitary gate with an arbitrary number of qubits. And thirdly, one applies these results to construct any unitary gate with one-qubit and CNOT gates.

1st Part. The proof of the first part is contained in the identity between quantum circuits shown in Fig. 28. In the lower part we show a controlled-unitary CU gate of two qubits associated to a unitary 2×2 matrix U . The upper part shows its decomposition in terms of one-qubit gates U_1, U_2, U_3, E and CNOT's. The rationale of this decomposition comes from group theory: any unitary 2×2 matrix U can be decomposed as

$$U = \text{Ph}(\delta)\bar{U}, \quad \bar{U} := R_z(\alpha)R_y(\beta)R_z(\gamma) \in \text{SU}(2) \quad (88)$$

where δ is the phase (mod π) of the $U(1)$ factor of $U(2)$, and α, β, γ are the Euler angles parameterizing the $\text{SU}(2)$ matrix \bar{U} . More explicitly,

$$\begin{aligned} \text{Ph}(\delta) &= \begin{pmatrix} e^{i\delta} & 0 \\ 0 & e^{i\delta} \end{pmatrix}, & R_z(\alpha) &= \begin{pmatrix} e^{-i\frac{\alpha}{2}} & 0 \\ 0 & e^{i\frac{\alpha}{2}} \end{pmatrix}, \\ R_y(\beta) &= \begin{pmatrix} \cos \frac{\beta}{2} & -\sin \frac{\beta}{2} \\ \sin \frac{\beta}{2} & \cos \frac{\beta}{2} \end{pmatrix}, & R_z(\gamma) &= \begin{pmatrix} e^{-i\frac{\gamma}{2}} & 0 \\ 0 & e^{i\frac{\gamma}{2}} \end{pmatrix}. \end{aligned} \quad (89)$$

With the help of this decomposition we can further show that for any unitary matrix \bar{U} in $\text{SU}(2)$ there exist matrices U_1, U_2, U_3 in $\text{SU}(2)$ such that

$$\begin{aligned} U_1 U_2 U_3 &= 1, \\ U_1 \sigma_x U_2 \sigma_x U_3 &= \bar{U}. \end{aligned} \quad (90)$$

The proof for this is by construction, namely,

$$\begin{aligned} U_1 &= R_z(\alpha)R_y(\tfrac{1}{2}\beta), \\ U_2 &= R_y(-\tfrac{1}{2}\beta)R_z(-\tfrac{1}{2}(\alpha + \gamma)), \\ U_3 &= R_z(\tfrac{1}{2}(-\alpha + \gamma)). \end{aligned} \quad (91)$$

Now, the equivalence between the quantum circuits of Fig. 28 proceeds by considering the two possibilities for the first qubit.

i) $|x_1\rangle = |0\rangle$. In this case the CNOT gates are not operative and using (90) we find that the second qubit $|x_2\rangle$ is not altered.

ii) $|x_1\rangle = |1\rangle$. In this case the CNOT gates do act on the second qubit producing altogether the chain of operations $\text{Ph}(\delta)U_1\sigma_x U_2\sigma_x U_3|x_2\rangle$, which using (90) turns out to be $U|x_2\rangle$. Recall that the controlled- σ_x gate is CNOT.

2nd Part. The proof of the second part is represented in Fig. 29 by another identity between quantum circuits. The proof is by induction on the number of qubits. We illustrate the simplest case. In the lower part we show a controlled-controlled-unitary C^2U^2 gate of three qubits associated to the square of an arbitrary unitary 2×2 matrix U . The upper part shows its decomposition in terms of controlled two-qubit gates (which in turn were already decomposed into one-qubit gates and CNOTs in the first part) and CNOTs.

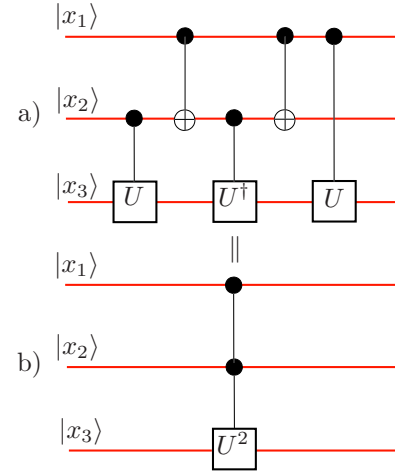


FIG. 29: Building-up a controlled-controlled- U^2 three-qubit gate from elementary gates.

The proof of this equivalence proceeds by considering the possible actions on the third qubit depending on the state of the other two qubits:

i) $|x_1\rangle = |0\rangle$. In this case, the two CNOT gates become inactive and so does the second controlled- U gate. We have two possibilities: a) if $|x_2\rangle = |0\rangle$ then neither of the remaining controlled gates operate and the net result is to leave $|x_3\rangle$ unchanged; b) if $|x_2\rangle = |1\rangle$ then the effect is now $U^\dagger U|x_3\rangle = |x_3\rangle$, as before.

ii) $|x_1 x_2\rangle = |10\rangle$. Now the CNOT gates do operate on the second qubit $|x_2\rangle$, and the second controlled- U gate acts on the third qubit. However, the first U -gate is inactive. Thus, the first CNOT gate changes the state of $|x_2\rangle$ to $|1\rangle$ and this makes the U^\dagger -gate become operative. Later, the action of the second CNOT brings the second qubit back to $|0\rangle$. Altogether, the final effect on $|x_3\rangle$ is

to yield $UU^\dagger|x_3\rangle = |x_3\rangle$, and remains unchanged again.

iii) $|x_1x_2\rangle = |11\rangle$. In this case we need to produce the action of U^2 on the third qubit. Now, all the gates in Fig. 29 become operative and we make a sequential counting of their effects. As $|x_2\rangle = |1\rangle$, the first U -gate does operate on the third qubit. Next, the action of the first CNOT gate sets $|x_2\rangle = |0\rangle$ so that the U^\dagger -gate becomes inactive. Then the second CNOT gate puts the second qubit back to $|1\rangle$. Altogether, the final effect on $|x_3\rangle$ is to yield $UU|x_3\rangle = U^2|x_3\rangle$, as required.

Finally, we can always choose the initial matrix U as the square root of a unitary matrix, say $U^2 = V$, such that the output in Fig. 29 is a C^2V -gate. For instance, if we choose $U = e^{i\pi/4}R_x(\frac{1}{2}\theta)$ we reproduce the Deutsch gate (82).

Moreover, we can go on and provide a construction of an arbitrary C^nV transformation (useful in quantum algorithms) by extending the construction in Fig. 29 to an arbitrary number of qubits. For instance, for a controlled- U^2 gate of 4 qubits we would have another qubit line on Fig. 29b) and then the construction holds by adding only a similar line to Fig. 29a) so that the two CNOT gates become CCNOT (C^2 NOT) gates and the last C^2U gate also picks up another control qubit gate. In general, for a n -qubit $C^{n-1}U^2$ gate that has $n-1$ control qubits and one target qubit where U^2 acts, the construction in Fig. 29 is generalized by simply using generalized C^{n-2} NOT gates with $n-2$ control qubits and a last $C^{n-1}U$ gate with $n-1$ control qubits. The proof of this generalized construction follows straightforwardly.

3rd Part. Combining finally the results in Parts 1 and 2 with the previously known construction of an arbitrary unitary matrix U as a product of two-level (not necessarily one-qubit) unitary matrices of Reck et al. (1994), one can easily represent U through one-qubit and CNOT gates, concluding this way the proof that *one-qubit gates plus CNOT is a set of elementary gates for exact universal computation* (Barenco et al., 1995).

So far we have only cared about the possibility of reconstructing a generic quantum gate from a given set of gates. The complexity of these constructions, measured by the number of basic gates necessary to achieve a certain gate simulation, is of great interest.

As an example of this issue, it is also interesting to count how many elementary gates in $\mathcal{G}_{\text{ex}}^{\text{II}}$ are needed to simulate a general C^nU gate. For instance, for a C^2U gate the first part of the proof yields 4 one-qubit gates and 2 CNOT's. For a generic controlled gate of n control qubits C^nU , the second part of the proof yields a quadratic dependence on n . To see this, let us denote by C_n the cost of simulating a C^nU gate. From the first part of the proof we know that the cost of simulating the U - and U^\dagger -gates in Fig. 29 is order $\Theta(1)$;⁴⁶ on the other hand, it is not difficult to show that the cost of the two

C^{n-1} NOTs is $\Theta(n+1)$ (Barenco et al., 1995). The cost of the generalized $C^{n-1}U$ gate is C_{n-1} , by recursive application of the recursive construction. Altogether, the cost of a gate satisfies a recursion relation like this

$$C_n = C_{n-1} + \Theta(n+1), \quad (92)$$

whose solution yields $C_n = \Theta((n+1)^2)$.

What is the size (number of gates) for exactly simulating an arbitrary gate of n qubits in $U(2^n)$? Barenco et al. (1995) showed that using the universal set $\mathcal{G}_{\text{ex}}^{\text{II}}$ this cost is $O(n^34^n)$;⁴⁷ Knill (1995) reduced this bound to $O(n4^n)$.

However, we are also interested in the efficiency of the approximate simulation of a generic gate. The universality property of a set of gates \mathcal{G}_{ap} means that, given an arbitrary quantum gate $U \in U(2^n)$ and $\epsilon > 0$, we can always devise an approximate quantum gate U' generated by \mathcal{G}_{ap} such that $d(U, U') < \epsilon$. The errors scale up linearly with the number of gates: given N gates U_i and their approximations U'_i , then the telescopic identity $U_1 \dots U_N - U'_1 \dots U'_N = \sum_{1 \leq k \leq N} U'_1 \dots U'_{k-1} (U_k - U'_k) U_{k+1} \dots U_N$ yields immediately $\|U_1 \dots U_N - U'_1 \dots U'_N\| < N\epsilon$.

This construction can be done efficiently using $\text{poly}(1/\epsilon)$ gates from the universal set (Lloyd, 1995; Preskill, 1998). Although we will not prove it, the underlying reason is simple: 1/ any universal set generates unitary matrices having eigenvalues with phases incommensurate relative to π ; 2/ if $\theta/\pi \in \mathbb{R}$ is irrational, then the integral powers $e^{ik\theta}$, $k \in \mathbb{Z}$ are dense in the unit circle S_1 , and given $\epsilon > 0$, any $e^{i\alpha} \in S_1$ is within a distance ϵ of some $e^{in\theta}$ with $n = O(1/\epsilon)$.

As a matter of fact, we can do much better than approximating a given n -qubit gate with circuits of size $\text{poly}(1/\epsilon)$ in the universal set \mathcal{G}_{ap} . A theorem of Solovay and Kitaev shows that it is possible an exponentially improved approximation (Solovay, 1995; Kitaev, 1997): Let \mathcal{G}_{ap} be an arbitrary finite universal set of gates, i.e. \mathcal{G}_{ap} generates a dense subset in $U(2^n)$. Then, any matrix $U \in U(2^n)$ can be approximated within an error ϵ by a product of $O(\text{poly}(\log(1/\epsilon)))$ gates in \mathcal{G}_{ap} (more precisely, $O(\text{poly}(\log(1/\epsilon))) = O(\log^c(1/\epsilon))$, with $c \approx 2$). The idea of the proof is to construct thinner and thinner nets of points in $U(2^n)$ by taking group commutators of unitaries in previous nets. It turns out that this way the width of the resulting nets decreases exponentially.

Finally, when the above Solovay-Kitaev theorem is combined with the complexity for exactly simulating gates with $\mathcal{G}_{\text{ex}}^{\text{II}}$, and the linearity of the error propagation with the number of gates, it immediately follows

$O(y)$ hold simultaneously.

⁴⁷The factor n^3 arises from the cost $O(n)$ to bring a generic two-level matrix to a C^{n-1} -unitary matrix which in turn costs $O(n^2)$. The dominant factor 4^n just counts asymptotically the maximum number of two-level unitary factors in the Reck et al. decomposition.

⁴⁶One writes $y = \Theta(x)$ to denote that both $y = O(x)$ and $x =$

that any unitary gate $U \in U(2^n)$ can be approximated to within error ϵ with $O(n4^n \log^c(n4^n/\epsilon))$ gates in any \mathcal{G}_{ap} . Note that this represents an exponential complexity in the number of qubits, i.e. most gates will be hard to simulate.

2. Arithmetics with QCs

The universality theorem of elementary quantum gates is a central result in the theory of quantum computation for it reduces the implementation of conditional quantum logic to a small set of simple operations. However, with a computer we are typically interested in doing arithmetic operations and thus we need to know how to perform quantum arithmetics with universal quantum gates. Vedral, Barenco and Ekert (1995) provided efficient ways of doing arithmetic operations such as addition, multiplication and modular exponentiation building on the Toffoli gate. The key point in their constructions is that we have to preserve the coherence of quantum states and make those operations reversible, unlike in a classical computer. For instance, the AND operation of Sec. VIII.D can be made reversible by embedding it into a Toffoli gate (Ekert, Hayden and Inamori, 2000): setting the third qubit to zero in (81) we get

$$U_{\text{CCNOT}}|x_1, x_2, x_3 = 0\rangle = |x_1, x_2, x_1 \wedge x_2\rangle. \quad (93)$$

Similarly, the quantum addition can be embedded into a Toffoli gate as shown in Fig. 30 with the help of a CNOT gate for the first two qubits. The result of the addition is stored in the second qubit.

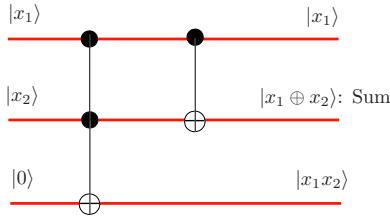


FIG. 30: The quantum addition from a Toffoli gate.

A quantum multiplication can be implemented in a similar fashion and also the exponentiation modulo N (Vedral, Barenco and Ekert, 1995). This latter operation is central in the Shor algorithm (Sec. X.D).

Another important operation that must be implemented in a quantum circuit is the evaluation of a function f . This must again comply with the requisite of reversibility, which is accomplished with a U_f -gate as shown in Fig. 31, where U_f is a unitary transformation that implements the action of f on certain qubits of the circuit. In this figure the box representing the evaluation of the gate is a kind of *black box*, also called *quantum oracle*, which represents the way in which we call or evaluate the function f . These evaluations are also called *queries*.

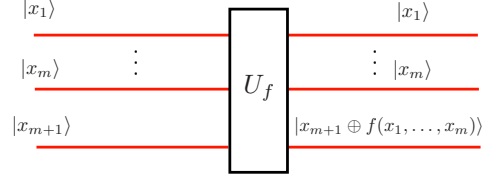


FIG. 31: A gate for function evaluation.

Reversible implementation of f requires to split the quantum register storing an initial state $|\Psi_0\rangle$ into two parts: the *source register* and the *target register*, namely,

$$|\Psi_0\rangle = |\Psi_s\rangle \otimes |\Psi_t\rangle, \quad (94)$$

where $|\Psi_s\rangle$ stores the input data for the computation and $|\Psi_t\rangle$ stores the output data, that is, the results of the quantum evolution or application of logic gates.

Thus, in order to implement a Boolean function $f : \{0,1\}^m \rightarrow \{0,1\}$ in a quantum circuit we need the action of a unitary gate U_f acting on the target register as follows

$$U_f|x_1x_2 \dots x_m\rangle_s |x_{m+1}\rangle_t = |x_1x_2 \dots x_m\rangle_s |x_{m+1} \oplus f(x_1, x_2, \dots, x_m)\rangle_t. \quad (95)$$

Why is it not possible to evaluate directly the action of f by a unitary operation that evolves $|x\rangle$ into $|f(x)\rangle$? The answer lies in unitarity of computation: we know that orthonormality is preserved under unitary transformations, thus if f is not a one-to-one mapping then two states $|x_1x_2 \dots x_m\rangle$ and $|x'_1x'_2 \dots x'_m\rangle$ that are initially orthonormal could evolve into two non-orthonormal states, say $|f(x_1, x_2, \dots, x_m)\rangle = |f(x'_1, x'_2, \dots, x'_m)\rangle$.

In the following we shall omit for simplicity the subscripts denoting source and target registers.

X. QUANTUM ALGORITHMS

In this section we present a survey of the most representative quantum algorithms to date, named after Deutsch-Jozsa, Simon, Grover and Shor, without entering the many spinoffs and ramifications that they have led to (Berstein and Vazirani, 1993; Hogg, 1998; Kitaev, 1995; etc.). We also use these quantum algorithms to emphasize and see in action the main ideas concerning the principles of quantum computation introduced in Sec. IX.

Due to space constraints, we have left out some interesting developments like *quantum clock synchronization*⁴⁸ (Chuang, 2000; Jozsa et al., 2000) and *quantum*

⁴⁸A way to make two atomic clocks start ticking at once. This can also be considered as an application of the quantum Fourier transform (see Sec. X.D for quantum phase estimation (Cleve et al., 1998))

The merging of Quantum Mechanics and Information Theory has proved to be very fruitful. One of the products of this is the discovery of quantum algorithms that outperform classical ones. It is appealing to think that the outcome of this merging is the fact that we can take classical algorithms and devise quantization processes in order to discover new modified quantized versions of classical algorithms. By quantizing a classical algorithm it is simply meant the possibility of using quantum bits in a quantum computer as opposed to the classical bits, and all the consequences thereof. This way of thinking is reminiscent of a well-known procedure of studying a quantum system by starting with its classical analogue and making a quantization of it, using for instance Dirac's prescription. One instance of this proposal is Shor's algorithm (Sec. X.D). In fact, Shor's algorithm relies on its ability to find the period of a simple function in number theory. The known classical algorithms for this task are inefficient because, as mentioned in Sec. VI, they have sub-exponential complexity in the input length (unless hard information is supplied aside). However, when qubits are used to implement the common algorithm (we quantize it in our language), then the principles of quantum computation shorten the task to polynomial time. Of this drastic improvement are responsible the peculiar properties of the discrete quantum Fourier transform (Sec. X.D).

Shor's algorithm also illustrates another common feature of the quantum algorithms known so far: they are best suited to study global properties of a function or a sequence as a whole, like finding the period of a function, the median of a sequence, etc., and not individual details. When the value of the function is needed for a particular choice of the argument, no real advantage is gained: one has to extract it from the quantum superposition and this may generally require measuring many times on the output to compensate the low probability, exponentially small in the register length, of getting the desired result.

Let us point out that it is possible to give a unified picture of most of the forthcoming algorithms in terms of the *hidden subgroup problem*: to find a generating set for a subgroup K of a finitely generated group G , given a function $f : G \rightarrow X$, where X is a finite set and f is constant and distinct on the K -cosets. Some instances of this problem are the Deutsch-Jozsa, Simon and Shor algorithms (Mosca and Ekert, 1999; Boneh and Lipton, 1995). Likewise, one may profitably view the quantum computation process as a multiparticle quantum interference (Cleve et al., 1998). However, we have adhered to a more traditional and historical pathway of presenting these quantum algorithms.

A. Deutsch-Jozsa Algorithm

This is the quantum algorithm first introduced by Deutsch (1985), providing an explicit and concrete example of how a quantum computer can beat a classical computer. Later, it was extended to more complex situations by Deutsch and Jozsa (1992). We shall present first an improved version (Cleve et al., 1998) of this algorithm for the simplest case of a Boolean function of a single qubit.

Suppose we are given an oracle which upon request computes a function $f : \{0, 1\}^n \rightarrow \{0, 1\}$. No other information on f is available, just the *promise* or assumption that f is either constant (i.e. $\forall x_1, x_2 \in \{0, 1\}^n, f(x_1) = f(x_2)$) or *balanced* (in the sense that $\#f^{-1}(0) = \#f^{-1}(1)$, i.e. the numbers of arguments mapping to 0 and to 1 are equal). The problem is to ascertain whether f is constant or balanced with as few queries to the oracle as possible.

The result of the DJ algorithm is that we only need one query or function evaluation to determine the nature of f , while classically $2^{n-1} + 1$ consultations would be necessary in the worst case.

Let us see this first when $n = 1$. Now f is balanced iff $f(0) \neq f(1)$, and thus the promise is worthless. The quantum circuit in Fig. 32 implements the DJ algorithm, and embodies the following steps:

Step 1. An initial quantum register is prepared with two qubits in the state $|\Psi_1\rangle := |01\rangle$.

Step 2. The Hadamard gate (75) is applied bit-wise to this quantum register, producing the state

$$|\Psi_2\rangle := U_H|0\rangle \otimes U_H|1\rangle = \frac{1}{2}(|0\rangle + |1\rangle) \otimes (|0\rangle - |1\rangle). \quad (96)$$

Step 3. We query the f -oracle with the state $|\Psi_2\rangle$, and get the answer $|\Psi_3\rangle := U_f|\Psi_2\rangle$. Using (95) we readily find

$$\begin{aligned} |\Psi_3\rangle &= U_f \frac{1}{2} \sum_{x=0,1} |x\rangle (|0\rangle - |1\rangle) \\ &= \frac{1}{2} \sum_{x=0,1} (-1)^{f(x)} |x\rangle (|0\rangle - |1\rangle). \end{aligned} \quad (97)$$

Step 4. The Hadamard gate is applied again to the first qubit, what yields

$$\begin{aligned} |\Psi_4\rangle &:= \frac{1}{2} \sum_{x=0,1} (-1)^{f(x)} (U_H|x\rangle) (|0\rangle - |1\rangle) \\ &= \frac{1}{2^{3/2}} \sum_{x=0,1} [(-1)^{f(x)}|0\rangle + (-1)^{x+f(x)}|1\rangle] \otimes (|0\rangle - |1\rangle). \end{aligned} \quad (98)$$

Step 5. Finally, we measure (in the computational basis) the first qubit (the second qubit plays no role anymore). There are two possibilities: i) either f is constant, and then the first-qubit amplitude of $|1\rangle$ in (98) vanishes and we measure $|0\rangle$ with certainty; ii) or f is not constant and consequently it is balanced, in which case it is the amplitude of $|0\rangle$ in (98) which vanishes and we measure $|1\rangle$ with certainty.

⁴⁹Quantum games appear so far to be more related to quantum communication protocols (Sec. III) or to applications of the above quantum algorithms.

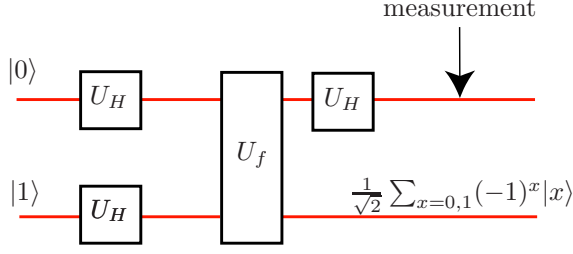


FIG. 32: Quantum circuit for the Deutsch-Jozsa algorithm.

Therefore, with this DJ algorithm we only need to call once the function in order to determine whether it is constant or balanced.

Let us point out how the peculiarities of quantum mechanics enter in the algorithm and provide its power. In step 2 it is possible to prepare a superposition of all the basis states using the Hadamard gates which have no classical analogue. In step 3 we evaluate the function on all the basis states at one go. However, this is not enough and we need to use interference of the quantum amplitudes in step 5 to discriminate between the two possibilities we were searching for. This is a simple manifestation of the idea of using constructive interference to distill the desired results as was already advanced in Sec. IX.A (see Table V).

The extension of the DJ algorithm to a function of n qubits $f : \{0,1\}^n \rightarrow \{0,1\}$ constrained to be either constant or balanced can be done with the help of the quantum circuit shown in Fig. 33. Following this circuit we can extend the previous 5 steps immediately. We prepare a source register with n qubits initialized to $|0\rangle$ and a target register with one qubit initialized to $|1\rangle$. With x we denote the integer $x := \sum_{i=0}^{n-1} x_i 2^i$ associated to the string of bits $x_{n-1} \dots x_1 x_0$, and $|x\rangle := |x_{n-1} \dots x_1 x_0\rangle$.

Let $|\Phi_1\rangle := |0\rangle|1\rangle$. After the bit-wise application of the Hadamard gate to $|\Phi_1\rangle$ we find

$$\begin{aligned} |\Phi_2\rangle &:= U_H^{\otimes(n+1)} |\Phi_1\rangle = (U_H|0\rangle)(U_H|0\rangle) \dots (U_H|0\rangle)(U_H|1\rangle) \\ &= \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} |x\rangle \frac{1}{\sqrt{2}} \sum_{y=0,1} (-1)^y |y\rangle. \end{aligned} \quad (99)$$

Using (95), the function evaluation on $|\Phi_2\rangle$ yields the following state

$$|\Phi_3\rangle := \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} (-1)^{f(x)} |x\rangle \frac{1}{\sqrt{2}} \sum_{y=0,1} (-1)^y |y\rangle. \quad (100)$$

In the next step we apply again the Hadamard gates but only on the n source qubits. After some algebra we

arrive at the final state $|\Phi_4\rangle$ given by

$$\begin{aligned} |\Phi_4\rangle &:= (U_H^{\otimes n} \otimes 1) |\Phi_3\rangle \\ &= \frac{1}{2^n} \sum_{x=0}^{2^n-1} \sum_{x'=0}^{2^n-1} (-1)^{x \cdot x' + f(x)} |x'\rangle \frac{1}{\sqrt{2}} \sum_{y=0,1} (-1)^y |y\rangle, \end{aligned} \quad (101)$$

where $x \cdot x' := \sum_{i=0}^{n-1} x_i x'_i \in \mathbb{Z}_2$.

If f is constant, then it produces an overall sign factor in (101), and after the double summation only the state $|x'\rangle = |0\rangle$ survives. On the contrary, if f is balanced, then the same reasoning shows that such state has zero amplitude in $|\Phi_4\rangle$. In summary, only when all the final source qubits are $|0\rangle$ the function is constant; otherwise, it is balanced.

Thus, measuring the state of the source qubits we can determine the nature of f with certainty.

This final measurement step allow us to take advantage of the interference among amplitudes obtained in previous stages.

A single query to the function black box has proved sufficient. However, with the classical algorithms known so far we would require a number of $2^{n-1} + 1$ function evaluations (in the worst case) to determine with certainty which type of function f is. This represents an exponential speed-up for this quantum algorithm.

Let us point out that classically, given any $1 > \epsilon > 0$, it is also possible to devise an efficient probabilistic algorithm such that running it a large enough number of times M (independent of the input length n) will determine whether any given function f is constant or balanced, with error probability $< \epsilon$. This is the procedure: the function f is evaluated for M random choices of the argument. When any two of the values differ, then we know that f is balanced. However, when all values are equal then the error probability in claiming that f is constant will be less than 2^{-M} . Thus, it suffices to choose M such that $2^{-M} < \epsilon$. In this sense, the quantum DJ algorithm is not such an impressive improvement over classical algorithms.

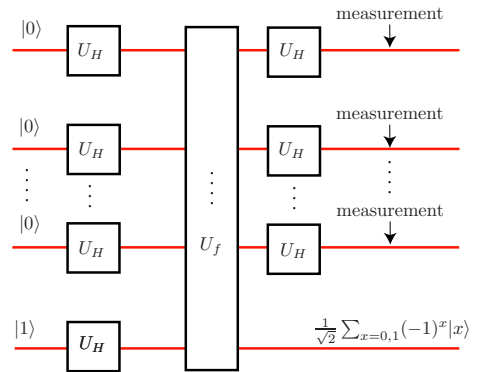


FIG. 33: Extended Deutsch-Jozsa algorithm.

B. Simon Algorithm

Simon's algorithm (1994) uses several tools of the DJ algorithm. It deals with a vector-valued Boolean function $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ which is constrained by the following condition or promise: There exists a non-null vector $p \in \{0, 1\}^n$, called the *period* of f , such that $f(x) = f(y)$ if and only if either $x = y$ or $x = y \oplus p$. Note that such an f is forcefully a 2-to-1 function.

This algorithm finds the period p after a number $O(n)$ of function evaluations, while the known classical algorithms would require an exponential number of queries.

The steps in Simon's algorithm can be seen in Fig. 34. Both the source and target registers have n qubits each. The algorithm proceeds as follows:⁵⁰

Step 1. The quantum registers are initialized to the state $|\Psi_1\rangle := |0\rangle|0\rangle = |00 \dots 0\rangle|00 \dots 0\rangle$.

Step 2. The Hadamard gate (75) is applied bit-wise to the source register, producing the state

$$|\Psi_2\rangle := (U_H|0\rangle) \dots (U_H|0\rangle)|0\rangle = \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} |x\rangle|0\rangle. \quad (102)$$

Step 3. The vector-valued function f is evaluated on the target qubits by applying the gate U_f . Using (95) we readily find the entangled state (Sec. III)

$$|\Psi_3\rangle := U_f|\Psi_2\rangle = \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} |x\rangle|f(x)\rangle. \quad (103)$$

Step 4. A further application of the Hadamard gates to the source qubits results in the state

$$\begin{aligned} |\Psi_4\rangle &:= \frac{1}{2^n} \sum_{x=0}^{2^n-1} \sum_{y=0}^{2^n-1} (-1)^{x \cdot y} |y\rangle|f(x)\rangle \\ &= \frac{1}{2^{n+1}} \sum_{x,y=0}^{2^n-1} [(-1)^{x \cdot y} + (-1)^{(x \oplus p) \cdot y}] |y\rangle|f(x)\rangle. \end{aligned} \quad (104)$$

Note that only those qubit states $|y\rangle$ such that $p \cdot y = 0$ enter with non-vanishing amplitudes in $|\Psi_4\rangle$. The remaining ones are washed out by destructive interference.

Step 5. An ideal measurement of the source qubits (in the computational basis) will necessarily yield a state $|y\rangle$ such that $p \cdot y = 0$ with probability $2^{-(n-1)}$.

Step 6. Repeating the previous steps M times we will get M vectors $y_{(i)}$ such that

$$p \cdot y_{(i)} = 0, \quad i = 1, \dots, M. \quad (105)$$

Solving this linear system with the Gaussian elimination algorithm will yield the period p with probability large enough provided $M = O(n)$.

⁵⁰Sometimes one introduces, for didactical purposes, a further step in which the target qubits are measured (Jozsa, 1997).

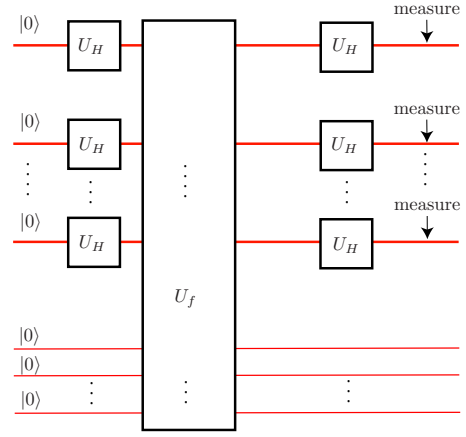


FIG. 34: Quantum circuit for Simon's algorithm.

The cost of Simon's algorithm is $O(n^2 + nC_f(n))$, where $C_f(n)$ is the cost of evaluating the function f on inputs of length n . The term n^2 is just the cost of the Gaussian elimination over \mathbb{Z}_2 .

However, a classical blind search would require $2^{n-1} + 1$ calls to the oracle in the worst case, and on the average a number $O(2^{n/2})$ of function evaluations (Shor, 2000). Thus, Simon's algorithm represents an exponential speed-up.

We note in passing that Simon's algorithm resorts to a classical algorithm (Gaussian elimination) to finish off the job. We shall find another interesting collaboration between quantum and classical procedures in Shor's algorithm.

C. Grover Algorithm

The previous quantum algorithms show explicitly some instances where a quantum computer beats a classical computer, as was advanced in Sec. VIII.A devoted to quantum Turing machines. However, they also present several drawbacks:

i) *utility*: it is not clear what they are useful for in practical applications.

ii) *structure*: the searched functions are constrained to comply with certain promises. These are called *structured problems*. Thus, we may feel as if those constraints quantumly conspire in favor of the DJ and Simon algorithms.

Grover's algorithm (1996, 1997) represents an example of *unstructured problem*: one in which no assumptions are made about the function f under scrutiny. Thus, we can contrast classical and quantum algorithms on equal footing. Although it came after Shor's algorithm (1994), we present it first for it is quite related to the previous algorithms.

The algorithm by Grover solves the problem of searching an element in a list of N unsorted elements. For in-

stance, searching a database like a telephone book when we know the number but not the person's name. When the size of the database becomes very large it is known to be one of the basic problems in computational science (Knuth, 1975). The utility of one such algorithm is guaranteed. Classically, one may devise many strategies to perform that search, but if the elements in the list are randomly distributed, then we shall need to make $O(N)$ trials in order to have a high confidence of finding the desired element. Grover's quantum searching algorithm takes advantage of the quantum mechanical properties to perform the searching problem with an efficiency of order $O(\sqrt{N})$ (Grover, 1996; 1997).

Let us state the searching problem in terms of a list $\mathcal{L}[0, 1, \dots, N-1]$ with a number N of unsorted elements. We shall denote by x_0 the marked element in \mathcal{L} that we are looking for. The quantum mechanical solution of this searching problem goes through the preparation of a quantum register in a quantum computer to store the N items of our list. This will allow exploiting quantum parallelism. Thus, let us assume that our quantum registers are made of n source qubits so that $N = 2^n$. We shall also need a target qubit to store the output of function evaluations or calls.

To implement the quantum search we need to construct a unitary operation that discriminates between the marked item x_0 and the rest. The following function

$$f_{x_0}(x) := \begin{cases} 0 & \text{if } x \neq x_0, \\ 1 & \text{if } x = x_0, \end{cases} \quad (106)$$

and its corresponding unitary operation (95)

$$U_{f_{x_0}}|x\rangle|y\rangle = |x\rangle|y \oplus f_{x_0}(x)\rangle \quad (107)$$

will do the job. We shall need to count how many applications of this operation or oracle calls are needed to find the item. The rationale behind the Grover algorithm is: 1/ to start with a quantum register in a state where all the computational basis states are equally present; 2/ to apply several unitary transformations to produce an output state in which the probability of catching the marked state $|x_0\rangle$ is large enough.

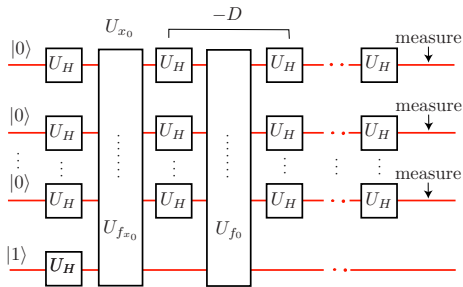


FIG. 35: The quantum circuit (up to an irrelevant global sign factor) for Grover's algorithm.

We present now the steps in Grover's algorithm, with the quantum circuit shown in Fig. 35.

Step 1. Initialize the quantum registers to the state $|\Psi_1\rangle := |00\dots 0\rangle|1\rangle$.

Step 2. Apply bit-wise the Hadamard one-qubit gate (75) to the source register, so as to produce a uniform superposition of basis states in the source register, and also to the target register:

$$|\Psi_2\rangle := U_H^{\otimes(n+1)}|\Psi_1\rangle = \frac{1}{2^{(n+1)/2}} \sum_{x=0}^{2^n-1} |x\rangle \sum_{y=0,1} (-1)^y |y\rangle. \quad (108)$$

Step 3. Apply now the operator $U_{f_{x_0}}$:

$$\begin{aligned} |\Psi_3\rangle &:= U_{f_{x_0}}|\Psi_2\rangle \\ &= 2^{-(n+1)/2} \sum_{x=0}^{2^n-1} (-1)^{f_{x_0}(x)} |x\rangle \sum_{y=0,1} (-1)^y |y\rangle. \end{aligned} \quad (109)$$

Let U_{x_0} be the operator defined by

$$U_{x_0}|x\rangle := (1 - 2|x_0\rangle\langle x_0|)|x\rangle = \begin{cases} -|x_0\rangle & \text{if } x = x_0, \\ |x\rangle & \text{if } x \neq x_0, \end{cases} \quad (110)$$

that is, it flips the amplitude of the marked state leaving the remaining source basis states unchanged. Grover presents this operator graphically as in Fig. 36, with a sort of “quantum comb” where the spikes denote the uniform amplitudes of state (108) and the action of U_{x_0} is to flip over the spike corresponding to the marked item.

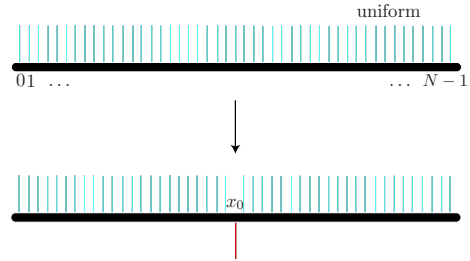


FIG. 36: Schematic representation of Grover's operator U_{x_0} in (110).

We realize that the state in the source register of (109) equals precisely the result of the action of U_{x_0} , i.e.

$$|\Psi_3\rangle = ([1 - 2|x_0\rangle\langle x_0|] \otimes 1)|\Psi_2\rangle. \quad (111)$$

Step 4. Apply next the operation D known as *inversion about the average* (Grover, 1996; 1997). This operator is defined as follows

$$D := -(U_H^{\otimes n} \otimes I)U_{f_0}(U_H^{\otimes n} \otimes I), \quad (112)$$

where U_{f_0} is the operator in (109) for $x_0 = 0$. The effect of this operator on the source qubits is to transform $\sum_x \alpha_x |x\rangle \mapsto \sum_x (-\alpha_x + 2\langle\alpha\rangle)|x\rangle$, where $\langle\alpha\rangle := 2^{-n} \sum_x \alpha_x$ is the mean of the amplitudes, so its net effect

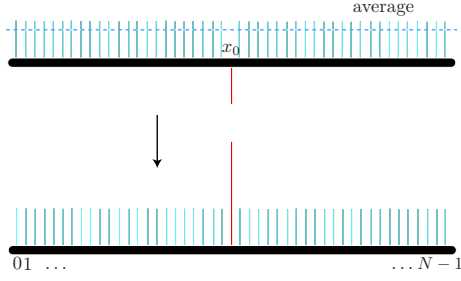


FIG. 37: Schematic representation of Grover's operator D in (112). The dashed line represents the mean amplitude.

is to amplify the amplitude of $|x_0\rangle$ over the rest. This is graphically represented in Fig. 37 (Grover, 1996; 1997).

Step 5. Iterate steps 3 and 4 a number of times m .

Step 6. Measure the source qubits (in the computational basis). The number m is determined such that the probability of finding the searched item x_0 is maximal.

The basic component of the algorithm is the quantum operation encoded in steps 3 and 4 which is repeatedly applied to the uniform state $|\Psi_2\rangle$ in order to find the marked element.

Although this procedure resembles the classical strategy, Grover's neatly designed operation enhances by constructive interference of quantum amplitudes (see Table V) the presence of the marked state one looks for.

It is possible to give a more general formulation to the operators entering steps 3 and 4 of the algorithm (Galindo and Martin-Delgado, 2000). To this end it is sufficient to focus on the source qubits and introduce the following definitions:

i) A *Grover operator* G is any unitary operator with at most two different eigenvalues; i.e., G a linear superposition of two orthogonal projectors P and Q :

$$G = \alpha P + \beta Q, \quad P^2 = P, \quad Q^2 = Q, \quad P + Q = 1, \quad (113)$$

where $\alpha, \beta \in \mathbb{C}$ are complex numbers of unit norm.

ii) A *Grover kernel* K is the product of two Grover operators:

$$K = G_2 G_1. \quad (114)$$

Some elementary properties follow immediately from these definitions:

a) Any Grover kernel K is a unitary operator.

b) Let the Grover operators G_1, G_2 be chosen such that

$$\begin{aligned} G_1 &= \alpha P_{x_0} + \beta Q_{x_0}, \quad P_{x_0} + Q_{x_0} = 1, \\ G_2 &= \gamma \bar{P} + \delta \bar{Q}, \quad \bar{P} + \bar{Q} = 1, \end{aligned} \quad (115)$$

with $P_{x_0} = |x_0\rangle\langle x_0|$, and \bar{P} given by the rank 1 matrix

$$\bar{P} := \frac{1}{N} \begin{pmatrix} 1 & \dots & 1 \\ \vdots & & \vdots \\ 1 & \dots & 1 \end{pmatrix}. \quad (116)$$

This is clearly a projector $\bar{P} = |k_0\rangle\langle k_0|$ on the subspace spanned by the state $|k_0\rangle = \frac{1}{\sqrt{N}}(1, \dots, 1)^t$, where the superscript denotes the transpose. Then, if we take the following set of parameters,

$$\alpha = -1, \quad \beta = 1, \quad \gamma = -1, \quad \delta = 1, \quad (117)$$

the Grover kernel (114) reproduces the original Grover's choice (1996; 1997). This property follows immediately by construction. In fact, we have in this case $G_1 = 1 - 2P_{x_0} =: G_{x_0}$ whilst the operator $G_2 = 1 - 2\bar{P}$ coincides (up to a sign) with the diffusion operator D (112) introduced by Grover to implement the inversion about the average of step 4.

The iterative part of the algorithm in step 5 corresponds to applying m times the Grover kernel K to the initial state $|x_{\text{in}}\rangle := 2^{-n/2} \sum_x |x\rangle$, which describes the source qubits after step 2, searching for a final state $|x_f\rangle$ of the form

$$|x_f\rangle := K^m |x_{\text{in}}\rangle, \quad (118)$$

such that the probability $p(x_0)$ of finding the marked state is above a given threshold value. We may take this value to be $1/2$, meaning that we choose a probability of success of 50% or larger. Thus, we are seeking under which circumstances the following condition

$$p(x_0) = |\langle x_0 | K^m | x_{\text{in}} \rangle|^2 \geq 1/2 \quad (119)$$

holds true.

The analysis of this probability gets simplified if we realize that the evolution associated to the searching problem can be mapped onto a reduced 2D-space spanned by the vectors

$$\{|x_0\rangle, |x_\perp\rangle\} := \frac{1}{\sqrt{N-1}} \sum_{x \neq x_0} |x\rangle. \quad (120)$$

Then we can easily compute the projections of the Grover operators G_1, G_2 in the reduced basis with the result

$$G_1 = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}, \quad (121)$$

$$G_2 = \begin{pmatrix} \delta & 0 \\ 0 & \gamma \end{pmatrix} + (\gamma - \delta) \begin{pmatrix} \frac{1}{N} & \frac{\sqrt{N-1}}{N} \\ \frac{\sqrt{N-1}}{N} & \frac{-1}{N} \end{pmatrix}. \quad (122)$$

From now on, we shall fix two of the phase parameters using the freedom we have to define each Grover factor in (114) up to an overall phase. Then we decide to fix them as follows:

$$\alpha = \gamma = -1. \quad (123)$$

With this choice, the Grover kernel (112) takes the following form in this basis:

$$K = \frac{1}{N} \begin{pmatrix} 1 + \delta(1-N) & -\beta(1+\delta)\sqrt{N-1} \\ (1+\delta)\sqrt{N-1} & \beta(1+\delta-N) \end{pmatrix}. \quad (124)$$

The source state $|x_{\text{in}}\rangle$ has the following components in the reduced basis

$$|x_{\text{in}}\rangle = \frac{1}{\sqrt{N}}|x_0\rangle + \sqrt{\frac{N-1}{N}}|x_{\perp}\rangle. \quad (125)$$

In order to compute the probability amplitude in (119), we introduce the spectral decomposition of the Grover kernel K in terms of its eigenvectors $\{|\kappa_1\rangle, |\kappa_2\rangle\}$, with eigenvalues $e^{i\omega_1}, e^{i\omega_2}$. Thus we have

$$a(x_0) := \langle x_0 | K^m | x_{\text{in}} \rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^2 \left\{ |\langle x_0 | \kappa_j \rangle|^2 + \sqrt{N-1} \langle x_0 | \kappa_j \rangle \langle \kappa_j | x_{\perp} \rangle \right\} e^{im\omega_j}. \quad (126)$$

This in turn can be cast into the following closed form:

$$\langle x_0 | K^m | x_{\text{in}} \rangle = e^{im\omega_1} \left(\frac{1}{\sqrt{N}} + (e^{im\Delta\omega} - 1) \langle x_0 | \kappa_2 \rangle \langle \kappa_2 | x_{\text{in}} \rangle \right), \quad (127)$$

with $\Delta\omega := \omega_2 - \omega_1$.

In terms of the matrix invariants

$$\text{Det}K = \beta\delta, \quad \text{Tr}K = -(\beta + \delta) + (1 + \beta)(1 + \delta) \frac{1}{N}, \quad (128)$$

the eigenvalues $\zeta_{1,2} := e^{i\omega_{1,2}}$ are given by

$$\zeta_{1,2} = \frac{1}{2} \text{Tr}K \mp \sqrt{-\text{Det}K + \frac{1}{4}(\text{Tr}K)^2}. \quad (129)$$

The corresponding unnormalized eigenvectors are

$$|\kappa_{1,2}\rangle \propto \begin{pmatrix} \frac{A \mp \sqrt{-4(\text{Det}K)N^2 + A^2}}{2(1+\delta)\sqrt{N-1}} \\ 1 \end{pmatrix}, \quad (130)$$

with

$$A := (\beta - \delta)N + (1 - \beta)(1 + \delta). \quad (131)$$

Although we could work out all the expressions for a generic value N of elements in the list, we shall restrict our analysis to the case of a large number of elements, $N \rightarrow \infty$ (see Fig. 38). Thus, in this asymptotic limit we need to know the behaviour for $N \gg 1$ of the eigenvector $|\kappa_2\rangle$, which turns out to be

$$|\kappa_2\rangle \propto \begin{pmatrix} \frac{\beta - \delta}{1 + \delta} \sqrt{N} + O\left(\frac{1}{\sqrt{N}}\right) \\ 1 \end{pmatrix}. \quad (132)$$

Thus, for generic values of β, δ we observe that the first component of the eigenvector dominates over the second one, meaning that asymptotically $|\kappa_2\rangle \sim |x_0\rangle$ and then $\langle x_0 | \kappa_2 \rangle \langle \kappa_2 | x_{\text{in}} \rangle = O\left(\frac{1}{\sqrt{N}}\right)$. This implies that the probability of success in (127) will never reach the threshold value (119). Then we are forced to tune the values of

the two parameters in order to have a well-defined and nontrivial algorithm, and we demand

$$\beta = \delta \neq -1. \quad (133)$$

Now the asymptotic behaviour of the eigenvector changes and is given by a balanced superposition of marked and unmarked states, as follows

$$|\kappa_2\rangle \sim \frac{1}{\sqrt{2}} \begin{pmatrix} i\delta^{1/2} \\ 1 \end{pmatrix}. \quad (134)$$

This is normalized and we see that none of the components dominates. When we insert this expression into (127) we find

$$|\langle x_0 | K^m | x_{\text{in}} \rangle| \sim \frac{1}{2} |\delta| |e^{im\Delta\omega} - 1| \sim \left| \sin\left(\frac{1}{2}m\Delta\omega\right) \right|. \quad (135)$$

This result means that we have succeeded in finding a class of algorithms which are appropriate for solving the quantum searching problem. Now we need to find out how efficient they are. To do this let us denote by M the smallest value of the time step m at which the probability becomes maximum; then, asymptotically,⁵¹

$$M \sim \lceil \pi / \Delta\omega \rceil. \quad (136)$$

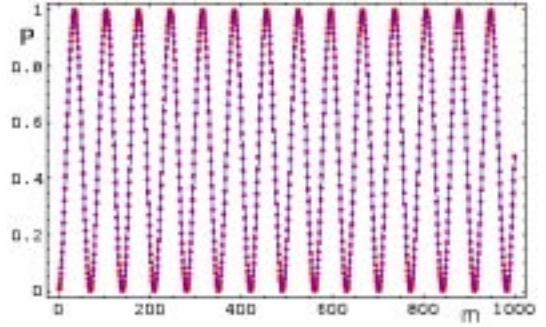


FIG. 38: Probability of success p as a function of the time step for $N = 1000$ and $\beta = \delta = e^{i\pi/2}$.

As it happens, we are interested in the asymptotic behaviour of this optimal period of time M . From the equation (129) we find the following behaviour as $N \rightarrow \infty$:

$$\Delta\omega \sim \frac{4}{\sqrt{N}} \text{Re}\sqrt{\delta}. \quad (137)$$

Thus, if we parameterize $\delta = e^{i\phi}$, then we finally obtain the expression

$$M \sim \left\lceil \frac{\pi}{4 \cos \frac{\phi}{2}} \sqrt{N} \right\rceil. \quad (138)$$

⁵¹The symbol $[x]$ stands for the closest integer to x .

Therefore, we conclude that the Grover algorithm of the class parameterized by ϕ is a well-defined quantum searching algorithm with an efficiency of order $O(\sqrt{N})$.

There have been many applications of Grover's work to quantum searching: finding the mean and median of a given set of values (Grover, 1996), searching the maximum/minimum (Durr and Hoyer, 1996), searching more than one marked item (Boyer et al., 1998), quantum counting, i.e., finding the number of marked items without caring about their location (Brassard, Hoyer and Tapp, 1998), etc. There is also a nice geometrical interpretation of the Grover kernel $K = -G_2 G_1$ in terms of two reflections G_1 and $-G_2$, one about $|x_\perp\rangle$ and the other about $|x_{\text{in}}\rangle$, producing a simple rotation of the initial state (Jozsa, 1999) by an angle $\theta = 2 \arcsin \frac{1}{\sqrt{N}}$ in the plane spanned by $|x_0\rangle$ and $|x_\perp\rangle$. With this construction it is straightforward to arrive at the following exact condition for the optimal value m of iterations:

$$m = \left\lceil \frac{1}{2} \left(\frac{\pi}{2 \arcsin \frac{1}{\sqrt{N}}} - 1 \right) \right\rceil. \quad (139)$$

Finally, it has been shown that Grover's algorithm is optimal (Bennett et al., 1997; Zalka, 1999), that is, its quadratic speed-up cannot be improved for unstructured lists.

D. Shor Algorithm

Shor's algorithm (1994) came as a wake-up call for cryptographers working with codes based on the difficulty of factoring large integer numbers⁵² (see Sec. VI.A), and now it represents a Damocles' sword hanging over this type of cryptosystems.

The algorithm of Shor has several parts that make it somewhat involved. It may be useful to keep in mind the main ingredients entering this algorithm:

- i) A periodic function.
- ii) Quantum parallelism.
- iii) Quantum Fourier transform.
- iv) Quantum measurement.
- v) Euclid's classical algorithm for finding the greatest common divisor $\gcd(n_1, n_2)$ of two integers n_1, n_2 .

Quantum computation opens the door to a new factorization method in polynomial time (Shor, 1994). This is why, although the technological difficulties to succeed in their construction are enormous,⁵³ it is highly interesting to find systems for key distribution whose security

(see Sec. VI.B) does not rely upon the practical difficulty of factoring large integers. Quite ironically, quantum physics provides both a fast factorization method and a secure key distribution (Sec. VI.B).

Let $N \geq 3$ be an odd integer to factorize. Let a be an integer in $(1, N)$. Let us assume that $\gcd(N, a) = 1$, that is, N and a are coprimes; otherwise $\gcd(N, a)$ would be a nontrivial factor f of N , and we would restart with N/f . The integral powers a^x of a form a cyclic group in $\mathbb{Z}_N := \mathbb{Z}/N\mathbb{Z}$, and there exists a smallest integer $r \in (1, N)$, called the *order* of a mod N , such that $a^r = 1$ in \mathbb{Z}_N . Several cases may arise:

- 1) r is odd;
- 2) r is even and $a^{r/2} = -1$ in \mathbb{Z}_N ;
- 3) r is even and $a^{r/2} \neq -1$ in \mathbb{Z}_N .

Only the case 3) is of interest for then $\gcd(N, a^{r/2} \pm 1)$ are nontrivial factors of N .

It can be shown that, for any given odd N , the probability of picking up at random an integer $a \in [1, N]$ coprime to N and fulfilling 3) is $\geq 1/(2 \log N)$, provided that N is not a pure prime power (Ekert and Jozsa, 1996).⁵⁴ Therefore it will be enough to analyze $O(\log(1/\epsilon) \log N)$ randomly chosen values of a to succeed in obtaining a nontrivial factor of N with a probability larger than $1 - \epsilon$. For example, if $N = 21823$, and $a = 12083$, the order of a mod N is $r = 3588$, and $12083^{1794} \equiv 4866 \pmod{21823}$, thereby $\gcd(12083^{1794} \mp 1, 21823) = \{139, 157\}$ are factors of 21823. On the contrary, although the order of $a = 14335 \pmod{N}$ is also even, namely $r = 1794$, however $14335^{897} \equiv -1 \pmod{21823}$, and $\gcd(14335^{897} \mp 1, 21823) = \{1, 21823\}$, so that no nontrivial factor of N is now obtained.

The big problem lies in computing the order r of a mod N for large N . And here is where the Shor algorithm comes in to quantumly search for the order r of an integer x in the multiplicative group \mathbb{Z}_N^* of integers modulo N , by producing a state with periodicity r .

As usual, we need two quantum registers: a source register with K qubits such that $Q := 2^K \in (N^2, 2N^2)$, and a target register with at least N basis states (i.e. with $\lceil \log_2 N \rceil$ qubits).

These are the main steps of Shor's algorithm (see Fig. 39):

Step 1. Initialize the source and target qubits to the state $|\Psi_1\rangle := |0\rangle \otimes |0\rangle$.

Step 2. Apply on the source register the *quantum Fourier transform* (which is just the discrete Fourier transform

⁵²“The problem of distinguishing prime numbers from composite numbers and of resolving the latter into their prime factors is known to be one of the most important and useful in arithmetic” (Gauss, 1801).

⁵³As Preskill (1997) recalls, it is quite risky to make guesses in this field; fifty years ago it was foreseen that “Where a calculator on the ENIAC is equipped with 18,000 vacuum tubes and weighs

30 tons, computers in the future may have only 1,000 tubes and perhaps only weigh 1 1/2 tons” (Popular Mechanics, March 1949), and the “future” has surpassed these expectations amply.

⁵⁴There are fast power tests to detect whether N is a prime power, say $N = p^s$, and to find p in that case (Cohen, 1993). A rudimentary transcendental and not very efficient procedure consists in trying with the integers $\lfloor N^{1/k} \rfloor, \lceil N^{1/k} \rceil, k = 2, 3, \dots, \lceil \log_2 N \rceil$, until hopefully finding one being a divisor of N .

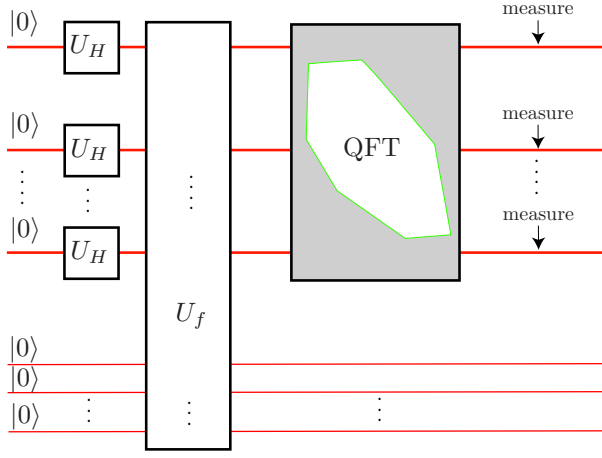


FIG. 39: A quantum circuit representing the Shor algorithm.

F_Q in \mathbb{Z}_Q):⁵⁵

$$U_{F_Q} : |q\rangle \mapsto \frac{1}{\sqrt{Q}} \sum_{q'=0}^{Q-1} e^{2\pi i q q' / Q} |q'\rangle. \quad (140)$$

Here, as usual, $q := \sum_{j=0}^{Q-1} q_j 2^j$, $q_j = 0, 1$, and $|q\rangle := |q_{Q-1} \dots q_1 q_0\rangle$. The following output state is produced:

$$|\Psi_2\rangle := (U_{F_Q} \otimes 1) |\Psi_1\rangle = Q^{-1/2} \sum_{q=0}^{Q-1} |q\rangle \otimes |0\rangle. \quad (141)$$

This particular case of the quantum Fourier transform corresponds to the Hadamard gate acting bit-wise on the source qubits.

Step 3. Next apply the gate U_a implementing the modular exponentiation function $q \mapsto a^q \bmod N$:

$$|\Psi_3\rangle := U_a |\Psi_2\rangle = Q^{-1/2} \sum_{q=0}^{Q-1} |q\rangle \otimes |a^q \bmod N\rangle. \quad (142)$$

This operation computes at one go $a^q \bmod N$ for all q as a manifestation of the quantum parallelism (see Sec. IX.A). *Step 4.* Apply again the Fourier transform U_{F_Q} on the source register. Then the state becomes

$$\begin{aligned} |\Psi_4\rangle &:= (U_{F_Q} \otimes 1) |\Psi_3\rangle \\ &= \frac{1}{Q} \sum_{q=0}^{Q-1} \sum_{q'=0}^{Q-1} e^{2\pi i q q' / Q} |q\rangle \otimes |a^{q'} \bmod N\rangle. \end{aligned} \quad (143)$$

Step 5. Measure the source qubits in the computational basis. The probability of finding them in the state $|q\rangle$ is

⁵⁵This is specially fast when $Q = 2^K$.

$\text{prob}(q) = \sum_{j=0}^{r-1} \text{prob}_j(q)$, where

$$\text{prob}_j(q) := \frac{1}{Q^2} \left| \sum_{k=0}^{B_j-1} \left(e^{2\pi i q r / Q} \right)^k \right|^2, \quad (144)$$

with $B_j := 1 + \lfloor (Q - 1 - j) / r \rfloor$.

To simplify the algebra, an intermediate step is introduced in most discussions of Shor's algorithm in which the target qubits are measured prior to the second application of the QFT (Shor, 1995; Ekert and Jozsa, 1996). If $|b\rangle$ is the result, the source register will be projected onto a state $B^{-1/2} \sum_{k=0}^{B-1} |d_b + kr\rangle$, superposition of basis states with the periodicity r of a^q . Here d_b is the minimum non-negative integer such that $a^{d_b} \bmod N = b$, and $B := 1 + \lfloor (Q - 1 - d_b) / r \rfloor$ is the length of the series. After applying the QFT and measuring the source qubits, the probability to obtain now $|q\rangle$ is just $(Q/B_{d_b}) \text{prob}_{d_b}(q)$.

Let us see how to pull out the order r of a from the study of the above probability $\text{prob}(q)$. The analysis of the geometrical series in (144) shows that $\text{prob}(q)$ peaks around those qs for which all the complex numbers in the sum fall in a same half-plane of \mathbb{C} , and thus they enhance each other constructively. It can be shown that such qs are characterized by $|(qr \bmod Q)| \leq \frac{1}{2}r$, they number r , and satisfy $\text{prob}(q) \geq (2/\pi)^2 r^{-1}$; therefore the probability of hitting upon anyone of them is $\geq (2/\pi)^2 = 0.405\dots$. In Fig. 40 the form of $\text{prob}(q)$ is shown.

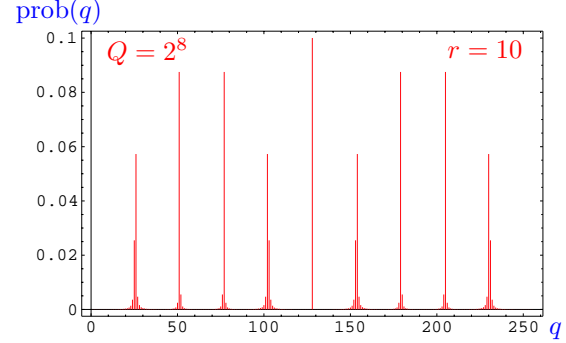


FIG. 40: The probability $\text{prob}(q)$ for the case $Q = 2^8$, $r = 10$. It gets concentrated around the integers $\lfloor sQ/r \rfloor$, with s integer.

The condition of constructive interference (see Table V) for each $q > 0$ amounts to the existence of an integer $q' \in (0, r)$ such that $|(q/Q) - (q'/r)| \leq \frac{1}{2}Q^{-1}$. As we have chosen $Q > N^2$, and $r < N$, there exists a unique q' such that the fraction q'/r satisfies that inequality. This rational number q'/r can be easily found as a convergent to the (finite simple) continued fraction expansion of q/Q . If this convergent is the irreducible fraction q_1/r_1 , it may happen that $a^{r_1} \equiv 1 \bmod N$, which implies $r = r_1$, and we are over. Otherwise, we would only know that r_1 is a divisor of r , and we would have to carry on, choosing another q with constructive

interference, to see if this time we are luckier. It can be shown that the probability of finding an appropriate q is order $\mathcal{O}(1/\log \log r)$, and therefore with a number $\mathcal{O}(\log \log N)$ of trials it is highly probable to obtain r .

For example, let be $N = 15$ (this is a sort of “toy model”), and $a = 7$. We can effortlessly see by brute force that $r = 4$. Suppose, however, that we insist in following the Shor way (quite a luxury in this case, but a necessity if N had half a thousand digits). We would take $Q = 2^8$ to comply with $N^2 < Q < 2N^2$. After step 5 we would obtain the state $|q\rangle$ of the source qubits, where, for instance, $q = 0, 64, 128, 192$ with probabilities $0.25, 0.25, 0.25, 0.25$. The first value is useless, for q/Q does not allow us to determine r if $q = 0$. From the continued fraction series expansion $\{a_0, a_1, a_2, \dots\} := a_0 + 1/(a_1 + 1/(a_2 + \dots))$ of q/Q ($64/256 = \{0, 4\}$, $128/256 = \{0, 2\}$, $192/256 = \{0, 1, 3\}$) we see that for $q = 64$ (resp. $128, 192$), the fraction $1/4$ (resp. $1/2, 3/4$) approximates q/Q with an error less than $1/2Q$. Thus, 4 is a divisor of r , i.e. $r = 4, 8, 12$, etc. A direct check selects $r = 4$ as the order of 7 mod 15. And since $7^{4/2} \not\equiv -1 \pmod{15}$, then $\gcd(49 \pm 1, 15) = \{5, 3\}$ are factors of 15.

As a little more complicated example, take $N = 25397, a = 71$. Then $Q = 2^{30} = 1073741824$. There are many values of q for which the probability is appreciable and similar. One of those is $q = 6170930$, for which $\text{prob}(q)$ is about 2×10^{-3} . The approximation $1/174$ to q/Q is the only convergent with denominator $< N$ provided us by the continued fraction expansion $\{0, 174, 1542732, 2\}$ of q/Q . Therefore, the order r of 71 mod 25397 is a multiple of 174, say $r = 174, 348, 522$, etc. A direct check shows that $r = 522$. Also in this case $a^{r/2} \not\equiv -1 \pmod{N}$, and $\gcd(71^{261} \pm 1, 25397) = \{109, 233\}$ are divisors of 25397.

In Fig. 41 the factorization time with an hypothetical quantum computer at 100 MHz is represented as a function of binary length of the integer to be factorized. The spectacular efficiency of the Shor algorithm stands out, with a time of 20 years for an integer of about 40 000 digits (Hughes, 1997).

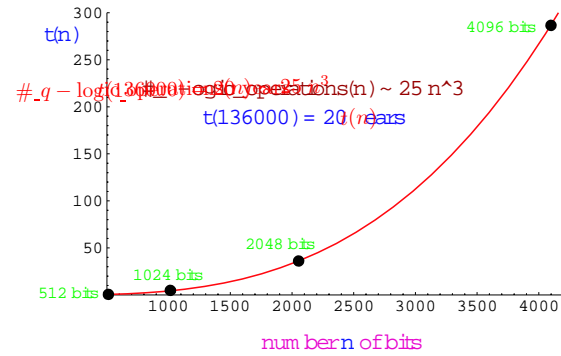


FIG. 41: Factorization times with a hypothetical QC at a nominal clock frequency of 100 MHz. The time $t(n)$, in minutes, is shown as a function of the number of bits.

Shor’s algorithm may seem a bit miraculous after those several “manipulations” or steps. The rationale is the same as described in Sec. IX: to drive the system into an appropriate outcome state that upon measurement yields the desired result with high probability. Where does the constructive interference ingredient (Table V) come into the algorithm? It is by means of the second QFT operation. This is designed to produce the interference among qubit amplitudes in such a way as to enhance those aspects of the output that favors the determination of the order r .

1. The Quantum Fourier Transform

Let us take a closer look at the discrete Fourier transform U_{F_Q} when $Q = 2^K$. It is at the core of Shor’s algorithm and is responsible for its exponential speed-up. To analyze the efficiency of the Shor algorithm it proves convenient to implement the QFT by means of one- and two-qubit gates. The result, shown in Fig. 42, will follow from the expression (140), duly worked out.

The phase factor $e^{2\pi i q q' / 2^K}$ in (140) is a periodic function of q , and of q' as well, with period 2^K . The numbers q and q' have the following binary decompositions: $q = \sum_{j=0}^{K-1} q_j 2^j$, $q_j = 0, 1$ and $q' = \sum_{l=0}^{K-1} q'_l 2^l$, $q'_l = 0, 1$. Then their product can be written as

$$qq' = \sum_{j,l=0}^{K-1} q_j q'_l 2^{j+l} = \sum_{0 \leq j+l < K} q_j q'_l 2^{j+l} \pmod{\mathbb{Z}_Q}. \quad (145)$$

By entering this expression into (140), and defining $\vec{q}'_l := q'_{K-1-l}$, $l = 0, \dots, K-1$, $0.abc\dots := 2^{-1}a + 2^{-2}b + 2^{-3}c + \dots$, we find

$$\begin{aligned} U_{F_Q} |q\rangle &= \frac{1}{\sqrt{Q}} \sum_{q'=0}^{Q-1} \exp(2\pi i q q' / 2^K) |q'\rangle \\ &= \frac{1}{\sqrt{Q}} \sum_{q'=0}^{Q-1} \exp(2\pi i \sum_{0 \leq j+l < K} q_j q'_l 2^{j+l-K}) |q'\rangle \\ &= \frac{1}{\sqrt{Q}} \sum_{\vec{q}'=0}^{Q-1} \exp(2\pi i \sum_{0 \leq j \leq l < K} q_j \vec{q}'_l 2^{j-l-1}) |\vec{q}'\rangle, \end{aligned} \quad (146)$$

and hence

$$\begin{aligned} U_{F_Q} |q\rangle &= \frac{1}{\sqrt{Q}} \sum_{\vec{q}'=0}^{Q-1} \bigotimes_{l=0}^{K-1} \exp(2\pi i \sum_{0 \leq j \leq l} q_j 2^{j-l-1} \vec{q}'_l) |\vec{q}'\rangle \\ &= \frac{1}{\sqrt{Q}} \bigotimes_{l=0}^{K-1} \sum_{\vec{q}'_l=0}^1 \exp(2\pi i \sum_{0 \leq j \leq l} q_j 2^{j-l-1} \vec{q}'_l) |\vec{q}'\rangle \\ &= \frac{1}{\sqrt{Q}} \bigotimes_{l=0}^{K-1} (|0\rangle + \exp(2\pi i 0.q_l q_{l-1} \dots q_0) |1\rangle). \end{aligned} \quad (147)$$

In particular, the transformed state $U_{F_Q}|q\rangle$ is separable. The QFT gate U_{F_Q} can be explicitly written as a product of Hadamard, controlled-phase and SWAP gates:

$$U_{F_Q} = \left(\prod_{i=0}^{\lfloor K/2 \rfloor - 1} U_{\text{SWAP}, i, K-1-i} \right) \times \prod_{l=K-1, \dots, 1, 0} \left(\left(\prod_{0 \leq j \leq l-1} U_{j, l}(\theta_{l-j}) \right) U_{H, l} \right), \quad (148)$$

where $\theta_j := \pi/2^j$, $U_{\text{SWAP}, i, j}$ exchanges the qubit states labelled by i, j , and

$$U_{H, l}|\dots q_l \dots\rangle := 2^{-1/2} \sum_{\vec{q}'_l=0,1} e^{i\pi q_l \vec{q}'_l} |\dots \vec{q}'_l \dots\rangle, \quad (149)$$

$$U_{j, l}(\theta)|\dots q_l \dots q_j \dots\rangle := e^{i q_l q_j \theta} |\dots q_l \dots q_j \dots\rangle$$

are the Hadamard gate action of the one-qubit $|q_l\rangle$, and the controlled-phase gate action on the two-qubit state $|q_l q_j\rangle$, respectively. From the factorization (148) we can read off the quantum circuit (see Fig. 42) implementing the QFT (up to a reversion of the output qubits).

The number of Hadamard gates in this implementation of the QFT is K , and that of the controlled-gates is $\frac{1}{2}K(K-1)$. Altogether this implies that the size of quantum circuit for Shor's algorithm is order $O(K^2)$ regardless of the SWAP gates for the final reversion (Coppersmith, 1994).⁵⁶

The quantum Fourier transform can be extended to deal with qubits with a number of states d not necessarily equal to 2 (see Sec. III). In this case the dimension of the Hilbert space of K source qubits is $Q = d^K$, and equations (140,149) for the QFT, the Hadamard and the controlled-phase gates hold true provided the phase angle is taken to be

$$\theta_j = \frac{2\pi}{d^{j+1}} \quad (150)$$

For instance, for qubits with $d = 3$ state or qutrits, the Hadamard gate takes the following explicit form

$$\begin{aligned} U_H^{(3)}|0\rangle &= \frac{1}{\sqrt{3}}[|0\rangle + |1\rangle + |2\rangle] \\ U_H^{(3)}|1\rangle &= \frac{1}{\sqrt{3}}[|0\rangle + \omega|1\rangle + \omega^2|2\rangle] \\ U_H^{(3)}|2\rangle &= \frac{1}{\sqrt{3}}[|0\rangle + \omega^2|1\rangle + \omega|2\rangle] \end{aligned} \quad (151)$$

with $\omega := e^{2\pi i/3}$.

⁵⁶In contrast, the classical fast Fourier transform requires order $O(K^2 K)$ elementary operations to transform a K -bit vector (Press et al., 1992).

In this general case, the sequence of one- and two-qubit gates for the decomposition of the QFT remains valid, as well as their counting. This implies that using qudits for QFT does not spoil its superb performance, while retaining the advantage of reducing by a factor of $\lfloor \log_2 d \rfloor$ the length of the quantum registers (see Sec. III).

2. Cost of Shor's Algorithm

We finally evaluate the complexity of Shor's algorithm. The first QFT transform (step 2) is just a Hadamard operation applied bit-wise and its cost is $O(\log_2 N)$. The modular exponentiation in step 3 consumes $O(\log_2^2 N \log_2 \log_2 N \log_2 \log_2 \log_2 N)$ time (Shor, 1994). The second QFT gate (step 4) is, according to the results just mentioned, $O(\log_2^2 N)$. Therefore the total cost to determine the order r of $a \bmod N$, with a probability of success $O(1)$, is $O(\log_2^{2+\epsilon} N)$, any $\epsilon > 0$.

Once r is determined, there remains to calculate $\gcd(a^{r/2} \pm 1, N)$ in order to find a factor of N . This arithmetical operation is more resource demanding, since it takes $O(\log_2^3 N)$ time steps when Euclid's celebrated algorithm is applied.⁵⁷

Altogether we end up with a total cost $O(\log_2^3 N)$ for the complete factorization algorithm with high probability,⁵⁸ what represents in practice a subexponential gain over the classical best algorithms (QS, GNFS) known nowadays.

E. On the Classification of Algorithms

One of the most important issues in quantum computing is the design of quantum algorithms. There are known very few of them. Apparently, we are lacking the basic principles underlying the quantum version of *algorithm problem solving*. We want in part to address this question and we believe that one attempt to understand the basic principles of quantum algorithm design may proceed with the comparison with the known strategies of designing classical algorithms in Computational Science. This is suggested by the studies about the relationships between fundamentals of classical and quantum computations presented in Sec. VIII and Sec. IX.A. In this regard, we need to distinguish between fundamentals of quantum computation and strategies for designing algorithms. Although the latter are still unknown, the former have been described in Table V. The fact that we can understand the fundamentals of quantum computation does not mean in principle that we know the keys to set up quantum algorithms, although it can be of great help.

⁵⁷Actually, a more refined implementation of the gcd algorithm (Knuth, 1981) reduces its cost to $O(\log N (\log \log N)^2 \log \log \log N)$.

⁵⁸Or better $O(\log_2^{2+\epsilon} N)$, if the previous footnote is considered.

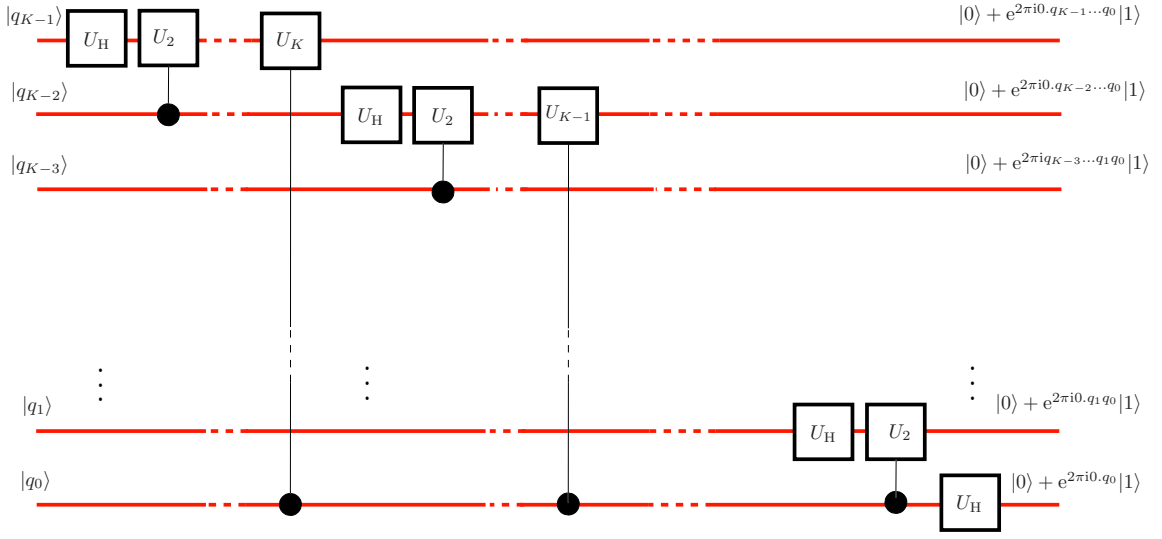


FIG. 42: Implementation of the quantum Fourier transform with Hadamard and controlled-phase gates (up to a reversion of output qubits). By U_j we denote the unary gate $U_j := |0\rangle\langle 0| + e^{2\pi i/2^j} |1\rangle\langle 1|$. For typographical reasons a factor $2^{-1/2}$ has been omitted in each output qubit.

Now let us come to the point of analysing the classical strategies of algorithm design from the point of view of quantum computation. To this end, we shall consider the classification introduced by Levitin (1999) who has done a reformulation which includes and categorizes in a nice fashion other classifications schemes (Brassard and Bratley, 1996). Following Levitin, there are four classical general design techniques which we shall describe briefly by its definition and with a simple example to illustrate them. This example is the problem of computing $a^n \bmod p$, which is of great importance in public-key encryption algorithms (Sec. VI, Sec. X.D). Then we have the following generic types:

1) *Brute Force Algorithms*

It amounts to solving a problem by directly applying its crude formulation. Example: $a^n = a \cdot a \cdots a$, n times.

2) *Divide-and-Conquer Algorithms*

The original problem is partitioned into a number of smaller subproblems, usually of the same kind. These in turn are then solved and their solutions combined to get a solution of the bigger problem. This strategy usually employs recursivity in order to obtain a greater profit. Example: $a^n = a^{\lfloor n/2 \rfloor} \cdot a^{\lfloor n/2 \rfloor} \cdot a^{n-2\lfloor n/2 \rfloor}$.

3) *Decrease-and-Conquer Algorithms*

The original problem is reduced to a smaller one, which is usually solved by recursion and the solution so obtained is applied to find a solution of the original problem. Examples: a) $a^n = a^{n-1} \cdot a$ (decrease-by-one variety); b) $a^n = (a^{\lfloor n/2 \rfloor})^2$ if n even, $a^n = (a^{\lfloor n/2 \rfloor})^2 \cdot a$ if n odd (decrease-by-half variety).

4) *Transform-and-Conquer Algorithms*

The original problem is transformed into another equivalent problem which is more amenable to solution with simpler techniques. Example: a^n is computed by

Classical Technique	Algorithm Example
Brute Force	Searching the Largest
Divide-and-Conquer	Quicksort
Decrease-and-Conquer	Euclid's Algorithm
Transform-and-Conquer	Gaussian Elimination

TABLE VIII: Classification of Classical Algorithms.

exploiting the binary representation of n .

These four types of strategies have in turn several subtypes we shall not dwell upon.

Table VIII contains these classical strategies with some well-known and less trivial examples of representative algorithms. There are important algorithms built upon a mixture of these basic techniques; for example, the Fast Fourier Transform employs both divide-and-conquer and transform-and-conquer techniques.

Now, it can be quite revealing to set up the quantum version of Table VIII by classifying the most useful of the so-far known quantum algorithms. This we do in Table IX.

Several remarks are in order.

Firstly, we have placed Grover's algorithm in the category of Brute Force algorithms. The strategy is similar to its classical counterpart, which is of Brute Force type. The difference lies in the fact that the quantum operation is realized through a unitary operator which implements the reversible quantum computation.⁵⁹ Although

⁵⁹By a similar rationale, we have placed Deutsch-Jozsa and Si-

Quantum Technique	Algorithm Example
Brute Force	Grover's Algorithm
	Deutsch-Jozsa' Algorithm
	Simon's Algorithm
Divide-and-Conquer	\emptyset
Decrease-and-Conquer	\emptyset
Transform-and-Conquer	Shor's Algorithm

TABLE IX: Classification of quantum algorithms.

the Brute Force technique gives usually low efficient algorithms, it is very important for several reasons. One is that there are important cases, like the searching problem, where the Brute Force method outperforms more sophisticated strategies like divide-and-conquer. We find Grover's algorithm as a realization of the Brute Force technique at the quantum level and this is why it is so simple and of general purpose at the same time.

Secondly, we have included Shor's algorithm in the category of transform-and-conquer algorithms. As we have explained in Sec. X.D, Shor solves the factorization problem by reducing it to the problem of finding the period of a certain function in number theory, which in turn is solved with the aid of the fundamentals of quantum computation. Having realized this, we point out that the classical version of transform-and-conquer algorithms are very rare (Anany, 1999). This may explain why Shor's algorithm, although more powerful than Grover's, it has a more reduced range of applications.

Thirdly, the most notorious aspect of Table IX is the absence of quantum algorithms based on the divide-and-conquer technique, which is by far the most general and used strategy in classical computation. This may partly account for the list of quantum algorithms being so short. Moreover, if we resort to the basic features of quantum computation (Table V) we may explain somehow why this entry is empty in Table IX. We know that a quantum register supports the superposition of many states at the same time. This implies that the qubits of the quantum registers are strongly correlated (entangled) and their joint state is not separable into a product of states of smaller subregisters. Thus quantum parallelism and entanglement render unnatural any try to implement the strategy of divide-and-conquer in a quantum register at least in a straightforward and naive fashion.⁶⁰

mon algorithms in the same class

⁶⁰A blend of classical and quantum algorithms might make room for a divide-and-conquer strategy.

XI. EXPERIMENTAL PROPOSALS OF QUANTUM COMPUTERS

The great challenge of quantum computation is to build real quantum computers capable of implementing the quantum logic operations of Sec. IX and of performing the quantum algorithms of Sec. X. In this section we present some of the experimental proposals to this end. Some of these proposals have been actually carried out, and this is already a significant advance for it means that the theoretical constructs can be checked experimentally. However, these devices are very modest in size and the real breakthrough will be to scale them up to sizes capable of doing tasks not yet done with classical computers, like code-breaking with Shor's algorithm or database searching with Grover's algorithm.

Before giving an overview of a few experimental proposals, it is convenient to summarize what they all have in common. There is a generic setting to build a quantum computer.⁶¹ We basically need:

- i) any two-level quantum system,
- ii) interaction between qubits,
- iii) external manipulation of qubits.

The two-level system is used as a qubit and the interaction between qubits is used to implement the conditional logic of the quantum logic gates (Sec. IX). The system of qubits must be accessible for external manipulations: to read in the input state and read out the output, as well as during the computation if the quantum algorithm requires it.

Interestingly enough, some of the possible qubits and quantum logic gates have been with us since the early times of Bohr. For example, the quantum NOT-gate is obtained, at least in principle, either by exciting an atomic ground state to an upper level with a photon of appropriate frequency and time length, or by induced emission. If the length of light pulses is halved, a Hadamard-like gate will result.⁶² Quantum computation has provided us with a new insight on these operations.

There are several settings in which one can illustrate the very basics of realizing experimental quantum computers and seeing the above three requirements in action. We shall choose as our qubit system a spin $\frac{1}{2}$ massive particle with magnetic moment, whose translational motion will be ignored.⁶³ Placing this qubit in a suitably oscillating external magnetic field will allow us to theoretically implement the unary quantum gates.

We shall not dwell upon all the practical technicalities of the experimental proposals below but instead present

⁶¹At least with our present knowledge.

⁶²Strictly speaking, this halved-pulse produces the action of the so-called *pseudo-Hadamard* gate.

⁶³Other simple choices are the polarization of a photon, an atomic system with just two relevant levels, etc.

the basic physical foundations underlying some of the quantum computers.

1. One- and Two-Qubit Logic Gates with Spin Qubits

This is one of the few examples where one can follow exactly the evolution of the quantum system, and it is versatile enough to let building some of the basic logic gates. We present it as a preparation for more complex setups.

Suppose that our qubit, a spin $\frac{1}{2}$ particle, has a magnetic moment $\boldsymbol{\mu} = \gamma \mathbf{S}$, where $\mathbf{S} = \frac{1}{2} \hbar \boldsymbol{\sigma}$ is the spin operator. In the presence of a uniform but time-dependent magnetic field $\mathbf{B}(t)$ the qubit state $|\psi(t)\rangle$ will evolve with the Hamiltonian $H(t) = -\gamma \mathbf{S} \cdot \mathbf{B}(t)$ (Rabi, 1937):

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = -\gamma \mathbf{S} \cdot \mathbf{B}(t) |\psi(t)\rangle. \quad (152)$$

When the magnetic field rotates uniformly around a fixed axis (say Oz), namely

$$\mathbf{B}(t) = (B_1 \cos \omega t, B_1 \sin \omega t, B_0), \quad (153)$$

then Eq. (152) can be solved explicitly, with the result (Galindo and Pascual, 1990b):

$$\begin{aligned} |\psi(t)\rangle &= U(t) |\psi(0)\rangle, \\ U(t) &:= e^{-i\omega t \sigma_z/2} e^{-i[(\omega_0 - \omega)\sigma_z + \omega_1 \sigma_x]t/2} = \\ &(\cos \tfrac{1}{2}\omega t - i(\sin \tfrac{1}{2}\omega t)\sigma_z)(\cos \tfrac{1}{2}\Omega t - i(\sin \tfrac{1}{2}\Omega t)\sigma'), \end{aligned} \quad (154)$$

where $\omega_0 := -\gamma B_0$, $\omega_1 = -\gamma B_1$, $\Omega := ((\omega_0 - \omega)^2 + \omega_1^2)^{1/2}$ is the so-called Rabi frequency, and $\sigma' := \Omega^{-1}[(\omega_0 - \omega)\sigma_z + \omega_1 \sigma_x]$.

As the computational basis (Sec. IX.A) we will take the eigenvectors of σ_z : $|0\rangle := |\uparrow\rangle$ (spin-up state), $|1\rangle := |\downarrow\rangle$ (spin-down state).⁶⁴

The probability of spin flip $\uparrow \leftrightarrow \downarrow$ is one if and only if $\omega = \omega_0$ (resonance condition), hence $\Omega = |\omega_1|$, and $t\Omega \in 2\pi(\mathbb{Z} + \frac{1}{2})$. When the oscillating part of the magnetic field (153) is resonant, i.e. it satisfies $\omega = \omega_0$, then such field is known as a *Rabi pulse*.

Let us see how to induce one-qubit operations using Rabi pulses of appropriate durations. In view of (88), and up to the global phase factor represented by $\text{Ph}(\delta)$ in (89), it suffices to do it for the rotations $R_z(\alpha)$, $R_y(\beta)$:

a) The rotation $R_z(\alpha)$ is emulated by taking a constant field along the z -axis and setting to zero the oscillating part ($B_1 = 0$, i.e. $\Omega = 0$). The angle is simply $\alpha = \frac{1}{2}\omega_0 T$, T being the pulse length. The rotation $R_z(\gamma)$ is obtained similarly.

b) To reproduce the rotation $R_y(\beta)$ in the decomposition (88), note that $R_y(\beta) = R_z(\frac{1}{2}\pi)R_x(\beta)R_z(-\frac{1}{2}\pi)$, and that $U(t) = R_z(\omega t)R_x(\Omega t)$. Therefore, to build $R_y(\beta)$ it suffices to compose with suitable rotations around Oz , implemented as above, the action of a Rabi pulse with $\Omega T = \beta$.

For instance, a π -pulse, i.e. a pulse with duration $T = \pi/\Omega$, reproduces in the interaction picture a quantum NOT-gate (up to a global factor -i).⁶⁵ Similarly, a $\frac{\pi}{2}$ -pulse produces essentially a Hadamard gate.

So far we have manipulated externally the spins $\frac{1}{2}$ to produce one-qubit gates. To generate two-qubit gates we need a pair of interacting qubits at sites 1, 2. For simplicity's sake, let us assume the simplest possible type of interaction between them, namely, an Ising interaction:

$$H_{12} = -(\gamma_1 S_1^z + \gamma_2 S_2^z)B^z + 2(J/\hbar)S_1^z S_2^z. \quad (155)$$

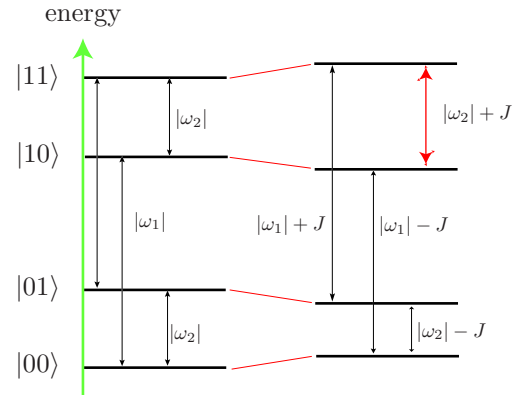


FIG. 43: Energy levels of a two-qubit spin system with Ising interaction (units $\hbar = 1$). On the left, the non-interacting Zeeman levels, and on the right the levels perturbed by the Ising term (when $\omega_1 < \omega_2 < -J < 0$).

The origin of the single spin terms may be the presence of an external magnetic field. In case (155), this field is constant and directed along Oz , and the two spins may have different magnetic moments. The coupling constant J measures the spin-spin interaction. Defining the frequencies $\omega_i := -\gamma_i B^z$, $i = 1, 2$, the eigenvalues of this Hamiltonian are

$$E_{x_1 x_2} = \frac{1}{2} \hbar [(-1)^{x_1} \omega_1 + (-1)^{x_2} \omega_2 + (-1)^{x_1 + x_2} J], \quad (156)$$

where $x_i = 0, 1$, $i = 1, 2$.

These energy levels are represented in Fig. 43 for $\omega_1 < \omega_2 < -J < 0$. We clearly see that if we apply a π -pulse with frequency $\omega = |\omega_2| + J$, the states $|11\rangle$ and

⁶⁴With this choice, $|0\rangle$ will be the ground state of the magnetic Hamiltonian provided that the spin corresponds to a positively charged particle ($\gamma > 0$).

⁶⁵At resonance, the time evolution operator $U(t)$ factorizes as $U(t) = e^{-i\omega_0 t \sigma_z/2} e^{-i\Omega t \sigma_x/2}$. The first factor represents the evolution operator $U_0(t)$ under the static magnetic field, whereas the second factor is just the total unitary propagator $U_I(t) := U_0^{-1}(t)U(t)$ in the interaction picture.

$|10\rangle$ get swapped while the rest are not excited. This is precisely what does a CNOT-gate with the first spin acting as control qubit and the second spin as a target qubit (Berman et al., 1997).

Other useful two-qubit gates such as the controlled-phase gate (78), that enters Shor's algorithm, can be built-up similarly using the Ising interaction. An explicit construction of this gate is the following (Jones, Hansen and Mosca, 1998)

$$U_{\text{CPh}}(\phi) = \exp\left(-i\frac{1}{2}\phi\left[-\frac{1}{2} + \bar{S}_1^z + \bar{S}_2^z - 2\bar{S}_1^z\bar{S}_2^z\right]\right), \quad (157)$$

where $\bar{S}_k^z := S_k^z/\hbar = \frac{1}{2}\sigma_k^z$. Of particular interest is the case $\phi = \pi$ for, as remarked in Sec. IX.B, with this controlled gate plus two Hadamard gates (on the target qubit) we can reconstruct the important CNOT gate (79).

A. The Ion-Trap QC

The ion-trap quantum computer was introduced by Cirac and Zoller (1995) and since then many other potential and actual realizations of quantum computers have been pursued by many groups. The quantum hardware is the following: a qubit is a single ion held in a trap by laser cooling and the application of appropriate electromagnetic fields; a quantum register is a linear array of ions; operations are effected by applying laser Rabi pulses; information transmission is achieved as a result of the Coulomb interaction between ions and the exchange of phonons from collective oscillations. We see again, at a very fundamental level, that information is physical. Using the Cirac-Zoller (CZ) technique it was possible to construct soon afterward a single quantum gate by Monroe et al. (1995).

The ion-trap proposal has several advantages: it needs manipulation of quantum states that were already known from precision spectroscopy techniques; it has low decoherence rates due to decay of excited states and the heating of the ionic motion; there exist very efficient experimental methods to retrieve the information from the quantum computer like the mechanism of quantum jumps.

1. Experimental setup

The geometry of a radio frequency (RF) ion-trap or Paul trap is schematically shown in Fig. 44. A RF Paul trap uses static and oscillating electric potentials to confine particles within small ($\sim 1 \mu\text{m}$) regions. To obtain a string of ions forming the quantum register we need a quadrupole ion trap with a cylindrical geometry. The confining mechanism of ions is twofold:

i) A strong *radial confinement*, achieved by RF potentials generally produced with four rod electrodes.

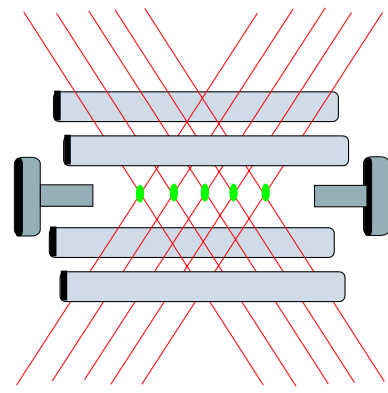


FIG. 44: Schematic geometry of a radio-frequency quadrupole linear ion-trap. Laser beams address a string of ions in the middle of the setup with 4 linear rods and 2 end-caps.

ii) An *axial confinement* achieved by applying a harmonic-like electrostatic potential through two end caps.

The ions lie along the trap axis and their oscillations are controlled by the axial potential. The collective oscillations of the string center of mass (CM) are used as a sort of computational bus, transferring information from one ion to another by phonon exchange. The dimensions of the ion-traps used by Los Alamos group are typically 1 cm long and 1-2 mm wide (Hughes et al., 1998).

Before any computation takes place, the CM of the ion string must be set to its ground state. This is accomplished by a laser cooling process that cools down the ions to the ground state of their vibrational motion. The result of this cooling is an ion string configuration as shown in Fig. 44, crystallizing into a linear array which makes possible to address each ion individually by lasers. The inter-ion spacing can be controlled as a balance of the ion Coulomb repulsion and the axially confining potential (Wineland et al., 1997).

Several kinds of ions (Be^+ , Ca^+ , Ba^+ , Mg^+ , Hg^+ , Sr^+ , etc.) and qubit schemes have been proposed. The CZ qubit $\{|0\rangle, |1\rangle\}$ is built using some appropriate electronic ion states. For instance, Los Alamos group (Hughes et al., 1998) have chosen Ca^+ ions, whose more relevant levels are shown in Fig. 45. The state qubits $\{|0\rangle, |1\rangle\}$ and one extra auxiliary level $|2\rangle$ (to be described below) are identified as follows (see Fig. 45):

$$\begin{aligned} |0\rangle &= |4^2S_{1/2}, M_J = \frac{1}{2}\rangle, \\ |1\rangle &= |3^2D_{5/2}, M_J = \frac{3}{2}\rangle, \\ |2\rangle &= |3^2D_{5/2}, M_J = -\frac{1}{2}\rangle. \end{aligned} \quad (158)$$

The level $(4^2S_{1/2}, M_J = \frac{1}{2})$ is the ground state while $(3^2D_{5/2}, M_J = \frac{3}{2})$ is a metastable level with a long lifetime (1.06 s). Both the electric-dipole transition $4^2S_{1/2} \rightarrow 4^2P_{1/2}$ at 397 nm wavelength and the electric quadrupole transition $4^2S_{1/2} \rightarrow 3^2D_{3/2}$ at 732 nm are

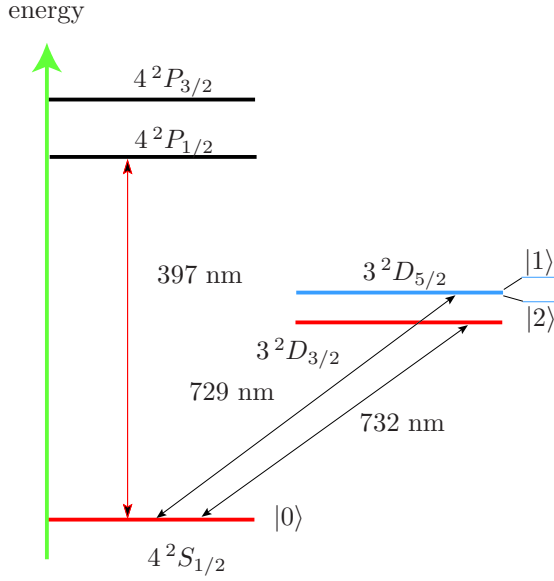


FIG. 45: Relevant energy levels in Ca^+ ions.

suitable for Doppler and sideband laser cooling, respectively. In Doppler cooling the laser radiation pressure slows down the axial motion of the ions until temperatures $T \sim$ a few mK. To further reduce the temperature ($T \sim$ a few μK) until no phonons are present, one resorts to sideband cooling (Hughes et al. 1997).

The interaction between CZ qubits is achieved using two types of degrees of freedom: internal (the electronic states of the ions), and external (the vibrational states of their collective excitations). Thus, an active state for information processing is the tensor product of an electronic state and a quantum oscillator state of the axial potential, namely,

$$|\Psi\rangle = |x\rangle|\alpha\rangle, x = 0, 1; \alpha = g, e, \quad (159)$$

where $|x\rangle$ refer to the electronic levels and $|g\rangle, |e\rangle$ denote the ground state and first excited state of the vibrational motion, respectively. In $|g\rangle$ there are no phonons present in the system while there is one phonon in $|e\rangle$ (see Fig. 46).

2. Laser pulses

With this structure of states one can apply two types of laser Rabi pulses to the ions in order to achieve quantum logic operations. These are called *V*- and *U*-pulses:

V-pulse. This pulse implements one-qubit operations. Its frequency is tuned to resonate with the optical transition between the qubit states. It swaps the electronic states $|0\rangle \leftrightarrow |1\rangle$ and leaves the vibrational mode in the ground state $|g\rangle$. The unitary evolution operator induced

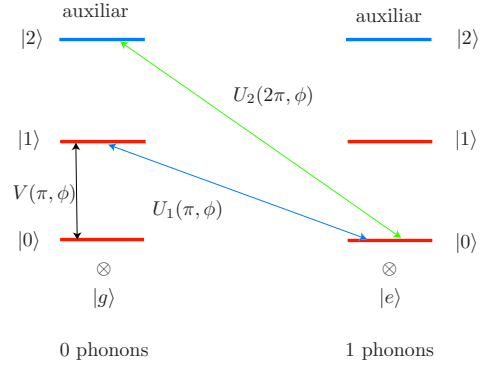


FIG. 46: Schematic representation of the transitions generated by the *V*- and *U*-pulses.

by this pulse is

$$V(\theta, \phi) := e^{-itH_V/\hbar}, \quad (160)$$

$$H_V := \frac{1}{2}\hbar\Omega[e^{-i\phi}|1\rangle\langle 0| + e^{i\phi}|0\rangle\langle 1|],$$

where $\theta := \Omega t$, H_V is the *V*-pulse Hamiltonian, Ω is the Rabi frequency (proportional to the square root of the laser intensity), and ϕ is the laser phase. Then, this pulse produces the following action on the electronic states:

$$V(\theta, \phi) : \begin{cases} |0\rangle \mapsto \cos\frac{\theta}{2}|0\rangle - ie^{-i\phi}\sin\frac{\theta}{2}|1\rangle, \\ |1\rangle \mapsto \cos\frac{\theta}{2}|1\rangle - ie^{i\phi}\sin\frac{\theta}{2}|0\rangle. \end{cases} \quad (161)$$

U-pulse. This pulse is used to implement two-qubit operations. The laser frequency is now adjusted to induce simultaneously both an electronic and a vibrational transition. To help performing the desired logic gates, an auxiliary electronic state $|2\rangle$ (see Fig. 46) is available. The time evolution operator led by this pulse is

$$U_{\hat{x}}(\kappa, \phi) := e^{-itH_U(\hat{x})/\hbar}, \quad \hat{x} = 1, 2, \quad (162)$$

$$H_U(\hat{x}) := \frac{1}{2}\hbar\eta\Omega[e^{-i\phi}|\hat{x}\rangle\langle 0| + e^{i\phi}|0\rangle\langle \hat{x}|],$$

where: H_U is the *U*-pulse Hamiltonian, $\kappa := \eta\Omega t$, η is the Lamb-Dicke parameter⁶⁶ and a^\dagger, a are creation and annihilation phonon operators satisfying

$$a^\dagger|g\rangle = |e\rangle, \quad a|e\rangle = |g\rangle, \quad [a, a^\dagger] = 1. \quad (163)$$

Several physical constraints on these parameters in a linear ion-trap are to be fulfilled for it to function stably and as required (Cirac and Zoller, 1995).

⁶⁶This quantity is the ratio between the width of the ion oscillation in the vibrational ground state of the register and the (reduced) laser wavelength $\lambda_L/2\pi$: $\eta := (\hbar/2NM_{\text{ion}}\omega_z)^{1/2}(2\pi/\lambda_L)$, where N is the number of cold ions, and ω_z is the vibrational frequency of the register CM along the trap axis. The Lamb-Dicke criterion $\eta \ll 1$ is demanded for Eq. (162) to be a good approximation (Cirac and Zoller, 1995). For the Ca^+ trap, with $N \sim 10$, $\omega_z \sim 100$ kHz, then $\eta \sim 0.2$.

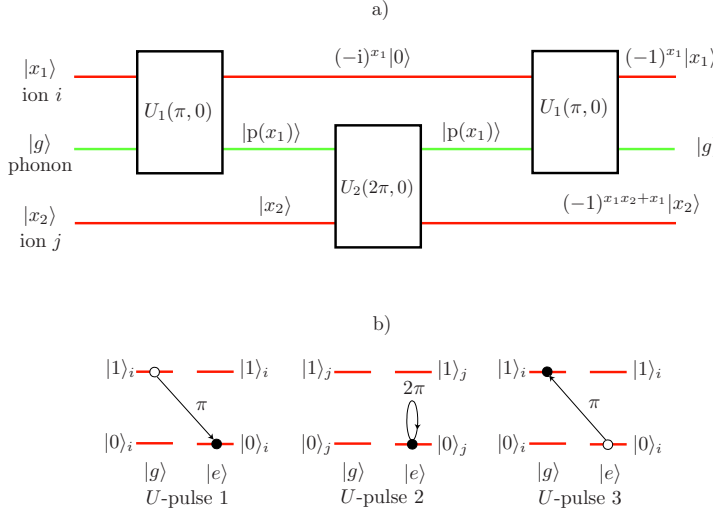


FIG. 47: a) Quantum circuit for the controlled-phase gate in an ion-trap QC. We denote by $|p(x_1)\rangle$ the phonon states $p(0) := g$, $p(1) := e$. Note also that the overall final phase is $(-1)^{x_1x_2}$, as it corresponds to a controlled phase $\phi = \pi$. b) Evolution of a state under the sequence of U -pulses in (165).

The U -pulse acts as follows:

$$U_{\hat{x}}(\kappa, \phi) : \begin{cases} |0\rangle|g\rangle \mapsto |0\rangle|g\rangle, \\ |0\rangle|e\rangle \mapsto \cos\frac{\kappa}{2}|0\rangle|e\rangle - ie^{-i\phi}\sin\frac{\kappa}{2}|\hat{x}\rangle|g\rangle, \\ |\hat{x}\rangle|g\rangle \mapsto \cos\frac{\kappa}{2}|\hat{x}\rangle|g\rangle - ie^{i\phi}\sin\frac{\kappa}{2}|0\rangle|e\rangle. \end{cases} \quad (164)$$

3. Building logic gates

By controlling the duration of the laser pulses in (161) and (164) we can perform logic operations in a fashion akin to those for spin qubits with Rabi pulses. The nice thing about the ion-trap QC is that the same Rabi pulses can drive conditional logic when phonons are suitably put to work.

For instance, a CNOT gate can be constructed using a series of V - and U -pulses. To this end, we first reproduce a π controlled-phase (78) gate between qubits at sites i, j as follows:

$$U_{\text{CPh}}^{(i,j)}(\pi) = U_1^{(i)}(\pi, 0)U_2^{(j)}(2\pi, 0)U_1^{(i)}(\pi, 0) \quad (165)$$

The explicit action of this sequence of operations is shown in Fig. 47. This two-bit gate is constructed only out of U -pulses.

In order to construct CNOT from this gate (see (79), Fig. 25) we need to resort to V -pulses, namely

$$U_{\text{CNOT}}^{(i,j)} = V^{(j)}(\frac{1}{2}\pi, \frac{1}{2}\pi)U_{\text{CPh}}^{(i,j)}(\pi)V^{(j)}(\frac{1}{2}\pi, \frac{1}{2}\pi) \quad (166)$$

where these V -pulses correspond to Hadamard gates. Other logic gates involving a larger number of qubits can

be constructed similarly using these basic pulse operations (Cirac and Zoller, 1995).

Let us note that the 2π auxiliary rotations in (165) do not produce any population of the auxiliary atomic levels nor the CM levels. Thus, a variation of the population of these levels by the gate operation would indicate a faulty experimental realization.

Upon completion of the quantum operations in the ion-trap QC, we need to readout the outcome result (see Sec. IX). This is done by measuring the state of each qubit in the quantum register using the quantum jump technique (Nagourney et al, 1986; Bergquist et al., 1986; Sauter et al., 1986). For instance, for the Ca^+ qubits (158), the laser is tuned to the dipole transition $4^2S_{1/2} \rightarrow 4^2P_{1/2}$ at 397 nm (see Fig. 45). Now, there are two possibilities for the ion being addressed with the laser: i) if the ion radiates (fluoresce), this means that its state is $|0\rangle$; ii) if the ion does not radiate (remains dark), then it was in the $|1\rangle$ state. Therefore, just by observing which ions fluoresce and which remain dark we can retrieve the bit values of the register. Actually, there is a third possibility in which $4^2P_{1/2} \rightarrow 3^2D_{3/2}$. In order to prevent this metastable level from being populated, a pump-out laser is also required.

4. Further applications

The ion-trap technique has also found applications in the preparation of entangled states (Molmer and Sorensen, 1999). This has been experimentally realized by the NIST group (Sackett et al., 2000) with the generation of entangled states of two and four trapped ions. In Fig. 48 a 4-qubit quantum register used in these experiments is shown.

Unavoidable errors put computational limits in ion-trap quantum computers. Sources of these constraints are the spontaneous decay of the metastable state, laser phase decoherence, ion heating and other kinds of errors. Using simple physical arguments it is possible to place upper bounds on the number of laser pulses N_U sustained by the ion trap before entering a decoherence regime (Hughes et al., 1996), namely,

$$N_UL^{1.84} < \frac{2Z(\tau/1\text{s})}{A^{1/2}F^{3/2}(\lambda/1\text{m})^{3/2}} \quad (167)$$

where Z is the ion degree of ionization, τ is the lifetime of the metastable state, L is the number of ions and A their atomic mass, F parameterizes the focusing capability of the laser and λ is the laser wavelength. This bound depends on the ion parameters A and τ , making some ion species more suitable than others.⁶⁷ With this

⁶⁷The number N_U refers only to the number U -pulses for they last much longer than the V -pulses, which are thus neglected.

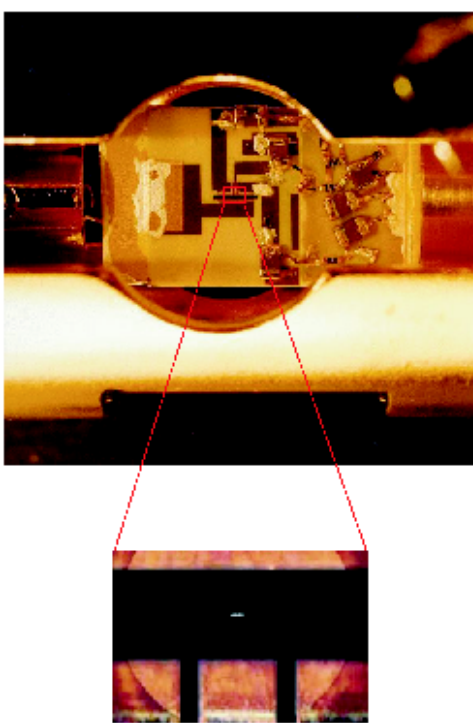


FIG. 48: Micromachined ion trap showing a four-qubit register in the inset (Sackett et al., 2000).

bound it is possible to estimate the number of ions needed to factorize a 438-bit number using Ytterbium (with the transition $4f^{14}6s^2 S_{1/2} \leftrightarrow 4f^{13}6s^2 {}^2F_{1/2}$, which has a very long lifetime (1533 days) and a wavelength of 467 nm). Around 2200 trapped ions and 4.5×10^{10} pulses would be required to perform the sought factorization, in about 100 hours of computation time (Hughes et al., 1996).

Scalability of the ion-trap QC is a central issue if we want to have a real useful machine for number factorization and the like. With current techniques, it is believed that prospects for reaching a few tens of qubits are good (Hughes et al., 1998). Cirac and Zoller (2000) have proposed an ion-trap based quantum computer with a two-dimensional array of independent ion traps and a different ion (head) that moves above this plane. This setup is still conceptually simple and it is believed to be within reach of present experimental technologies.

B. NMR Liquids: Quantum Ensemble Computation

We have seen that using spin qubits and spin resonance is a natural choice for doing quantum computations. Nuclear spins are good candidates for spin qubits but they pose both theoretical and experimental challenges. There have been independent proposals to overcome these difficulties: the *logical labelling formalism* by Gershenfeld, Chuang and Lloyd (1996), Gershenfeld and Chuang (1997), and the *spatial averaging formalism* by

Cory, Fahmy and Havel (1997). They have been addressed experimentally by several groups. Later, a *time averaging formalism* was introduced by Knill, Chuang and Laflamme (1997).

The quantum hardware in this case consists of a liquid containing a large number of molecules of a certain type. A qubit is the spin of a nucleus in a molecule, and a quantum register is a molecule as a whole, i.e., each molecule is an independent quantum computer; operations are effected using nuclear magnetic resonance techniques (Rabi oscillations) and information transmission between nuclei is based on the spin interactions within each molecule.

1. Spins at thermal equilibrium

The choice of nuclear spins as qubits has several pros and cons. On one hand, nuclear spins in a molecule of a liquid are very robust quantum systems, for they are well screened from other sources of magnetic fields by the electron cloud that surrounds them. This results in decoherence times of the order of seconds, long enough to let quantum computations going on. On the contrary, in a liquid at finite temperature the nuclear spins form a highly mixed state, not a pure state as we have been assuming in the formalism for quantum computation introduced so far. Such formalism needs be modified accordingly, by describing with *density matrices* the mixed states of spins and their evolution.

A consequence of the finite temperature is that the precise initial conditions of a particular nuclear spin are not known as required for standard quantum computation. Instead, we can only know the probability of finding the spin in one of the two states $|0\rangle = |\uparrow\rangle$ or $|1\rangle = |\downarrow\rangle$. In the following, we shall assume that the molecules in the solution are in thermal equilibrium at some temperature T . Hence the density matrix describing the quantum state of the relevant nuclear spins in each single molecule is

$$\rho := \frac{e^{-\beta H}}{\text{Tr}[e^{-\beta H}]}, \quad (168)$$

where H is the Hamiltonian of the system, $\beta = 1/k_B T$ the inverse temperature, and the trace is over any orthonormal basis of the Hilbert space. Let us take the simplest case of a single spin qubit with a Zeeman splitting Hamiltonian $H = \omega S^z$, $\omega = -\gamma B_0$. Then, (168) becomes

$$\begin{aligned} \rho_{00} &= \frac{e^{-\beta \hbar \omega / 2}}{e^{\beta \hbar \omega / 2} + e^{-\beta \hbar \omega / 2}}, \\ \rho_{11} &= \frac{e^{\beta \hbar \omega / 2}}{e^{\beta \hbar \omega / 2} + e^{-\beta \hbar \omega / 2}}, \\ \rho_{01} &= 0 = \rho_{10}. \end{aligned} \quad (169)$$

The diagonal terms of ρ represent the probability of finding the spin in the state $|0\rangle$ or $|1\rangle$. In contrast, the density

matrix of a pure state $|\psi(t)\rangle := \alpha_0(t)|0\rangle + \alpha_1(t)|1\rangle$ is

$$\rho_\psi := |\psi\rangle\langle\psi| = \begin{pmatrix} |\alpha_0|^2 & \alpha_0\alpha_1^* \\ \alpha_0^*\alpha_1 & |\alpha_1|^2 \end{pmatrix}. \quad (170)$$

Therefore we see that at finite temperature and thermal equilibrium, the off-diagonal elements of the density matrix average to zero while they are non-vanishing for a generic pure quantum state.

2. Liquid state NMR spectroscopy

To overcome these difficulties, the proposal for a NMR quantum computer takes advantage of the highly developed techniques in liquid state NMR spectroscopy accumulated for fifty years (Ernst et al., 1987).

In a NMR liquid the molecules are in solution. In each molecule only some of its nuclei are active for doing quantum computation. When the qubits consist of atomic nuclei of the same chemical element the molecules are called *homonuclear*, and *heteronuclear* otherwise. Examples of homonuclear molecules are shown in Fig. 49, like the 2,3-dibromo-thiophene where the active nuclear spins are those of the two Hydrogen atoms, or the 1-chloro-2-nitro-benzene with four active Hydrogen atoms. An example of heteronuclear molecule is the ^{13}C -labelled chloroform⁶⁸ in which the two active qubits come from the atoms of Hydrogen and Carbon. The number of qubits in the working register narrows the choice of the molecule structure.

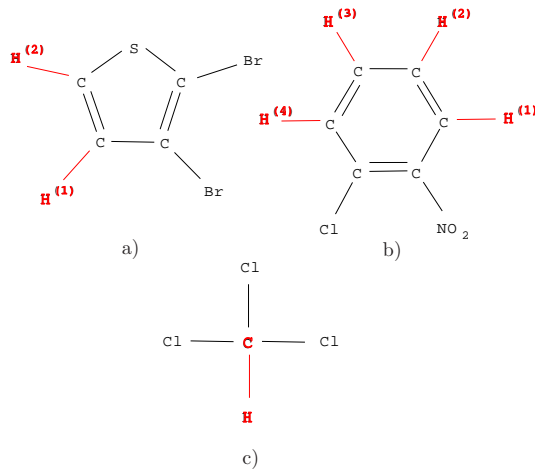


FIG. 49: Some examples of molecules used in NMR liquid quantum computation: a) 2,3-dibromo-thiophene (homonuclear), b) 1-chloro-2-nitro-benzene (homonuclear), c) chloroform (heteronuclear)

⁶⁸The nucleus of the most common isotope ^{12}C is spinless. Adding one extra neutron endows it with an overall operative spin $\frac{1}{2}$.

An appropriate experimental setup for NMR computation is much like any other instrumentation used in NMR spectroscopy. In Fig. 50 the basic structure of a NMR spectrometer is shown. The liquid sample is held in a probe inside a radio-frequency cavity subjected to a strong homogeneous magnetic field of around 10 T, usually produced by a superconducting magnet. The RF cavity is tuned to the resonance frequencies of the active nuclear spins.

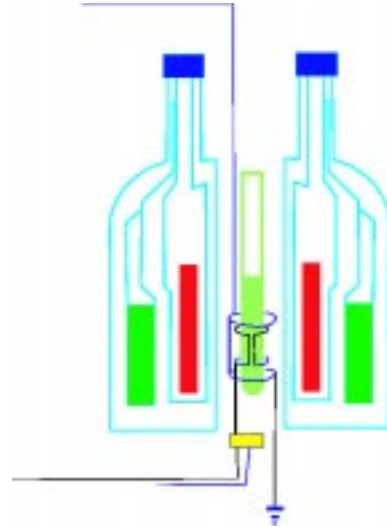


FIG. 50: Schematic setup of a NMR experiment

In a typical sample there are $N \sim 10^{18}$ molecules in solution. The dipole-dipole interactions between the spins in different molecules as well as other intermolecular interactions average to zero due to the random rotational motion of the molecules in the usual time scale for controlling the spin dynamics and the measurement (Slichter, 1990). Hence, only interactions within each molecule are observable and the sample can be regarded as an ensemble of independent and mutually incoherent quantum computers. This reasonable approximation yields a huge reduction in the large density matrix of dimension $\sim 2^{O(N)}$ describing the whole ensemble of active nuclear spins, which may be replaced by a much smaller density matrix of dimension 2^n , where n is the number of active nuclei in a single molecule.

Within each molecule, the total Hamiltonian $H(t)$ of the active spins has two parts (Cory et al., 2000), one internal and another external:

$$H(t) := H_{\text{int}} + H_{\text{ext}}(t). \quad (171)$$

The internal Hamiltonian describes the interactions among spins within the molecule, while the external Hamiltonian controls the spin dynamics under Rabi pulses. The operator H_{int} embodies: a) the molecule interaction energy with a strong homogeneous magnetic field that causes a Zeeman splitting of the nuclear spin

levels; b) the spin-spin interactions between active nuclei, modelled by a magnetic exchange interaction $2(J_{ij}/\hbar)\mathbf{S}_i \cdot \mathbf{S}_j$ mediated by electrons in molecular orbitals that overlap both nuclear spins i, j . In most cases this interaction can be further simplified using the weak coupling approximation $|J_{ij}| \ll |\omega_i - \omega_j|$, which assumes that the spin-spin coupling is much smaller than the Zeeman splitting. This simplification produces a *scalar coupling* of Ising type between the spins, and yields the following good approximation to the internal Hamiltonian:

$$H_{\text{int}} \approx \sum_{i=1}^n \omega_i S_i^z + 2 \sum_{i \neq j=1}^n (J_{ij}/\hbar) S_i^z S_j^z, \quad (172)$$

where J_{ij} measures the coupling between the active spins at sites i, j ,⁶⁹ and ω_i are the resonance frequencies for each spin. They are different even for homonuclear molecules due to the unlike screening of each nuclear spin from the surrounding electrons. This effect is called *chemical shift*. Thus, in (172) the one-body terms may be used to distinguish qubits, while the two-body terms serve to implement the conditional logic of two-qubit gates. The values of the parameters ω_i and J_{ij} are determined by standard NMR spectroscopy techniques prior to the computation. Standard NMR spectroscopy and NMR quantum computation share the means but differ in goals: in the former we aim to determine the parameters of the Hamiltonian (172) to study the chemistry and dynamics of the molecules in solution, while in the latter the form of (172) is already known and we set out to use it to perform controlled logic operations.

The external time dependent Hamiltonian $H_{\text{ext}}(t)$ helps to control the evolution of the spins. These form an ensemble of systems, initially described by the thermal density matrix ρ (169) and its time evolution is

$$\rho(t) = U(t)\rho(0)U^\dagger(t), \quad (173)$$

where $U(t)$ is the unitary propagator generated by the total Hamiltonian in (171) and $\rho(0)$ is the thermal density matrix (169).

3. High temperature regime: pseudo-pure states

The evolution of the density matrix (168) is simplified in the high temperature limit $k_B T \gg \hbar \omega_i$, where the Zeeman splittings are much smaller than the Boltzmann energy. Then, we can approximate (168) as follows

$$\rho \simeq \frac{1 - \beta H}{\text{Tr}(1 - \beta H)} \simeq \rho_n := \frac{1}{2^n} - \frac{\beta H}{2^n}. \quad (174)$$

Thus, in NMR quantum computing there is no need for cooling down the system until reaching its ground state as in other types of QCs.

Let us analyze step by step the approximation (174) for quantum computing. First, let us consider the case of a single spin. Then, the density matrix is simply given by

$$\begin{aligned} \rho_1 &:= \frac{1}{2} - \epsilon_1 \delta_1, \\ \delta_1 &:= \bar{S}_1^z, \quad \epsilon_1 := \frac{1}{2} \hbar \omega_1 / k_B T, \end{aligned} \quad (175)$$

where δ_1 is called the *deviation density matrix*⁷⁰ and $|\epsilon_1| \sim 10^{-5}$ at room temperature for conventional NMR liquids. Thus, the factor ϵ_1 gives the strength of the NMR signal relative to background noise. This expression can be further simplified by dropping out the unit term, which does not change under time evolution (173): in a NMR experiment the expectation value of an observable O is given by

$$\langle O \rangle = \text{Tr}(O\rho), \quad (176)$$

and, as it happens, all NMR observables are traceless. Thus, all the information is in $\epsilon_1 \delta_1$. As ϵ_1 enters only as an overall scale factor, we can also drop it out in all this description and write the effective thermal density matrix simply as

$$\rho_1 \sim \bar{S}_1^z. \quad (177)$$

Now let us recall that for a qubit in the ground state or excited state the density matrices are

$$\begin{aligned} \rho_{|0\rangle} &= |0\rangle\langle 0| = \frac{1}{2} + \bar{S}^z, \\ \rho_{|1\rangle} &= |1\rangle\langle 1| = \frac{1}{2} - \bar{S}^z, \end{aligned} \quad (178)$$

and discarding the unit terms, we see that for NMR purposes the one-qubit states $|0\rangle, |1\rangle$, are equivalent to $\bar{S}^z, -\bar{S}^z$, respectively. The spin operators representing one-qubit states in this correspondence are called *pseudo-pure* or *effective pure states*. It also works for a superposition state; for instance, the pure state $|\Psi\rangle = 2^{-1/2}(|0\rangle + |1\rangle)$ has a density matrix

$$\rho_{|\Psi\rangle} = \frac{1}{2} + \bar{S}^x, \quad (179)$$

equivalent to \bar{S}^x . Actually, the correspondence is one-to-one in the case of one-qubit states, for the density matrix of a single pure state (170) is a Hermitean operator that can be expanded as a real linear combination of the Pauli matrices $\{1, \sigma^x, \sigma^y, \sigma^z\}$.

Then, the time evolution of a NMR density matrix is that of the spin $\frac{1}{2}$ operators. When the external Hamiltonian corresponds to a Rabi pulse, the transformation laws are simple. The evolution operator for a single spin with Zeeman Hamiltonian $H_1 := \hbar \omega_1 \bar{S}_1^z$ is

$$U_Z(t) := e^{-it\omega_1 \bar{S}_1^z} = \cos(\frac{1}{2}\omega_1 t)1 - 2i \sin(\frac{1}{2}\omega_1 t)\bar{S}_1^z, \quad (180)$$

⁶⁹In NMR spectroscopy J_{ij} are typically ~ 100 Hz.

⁷⁰Sometimes it is also called *reduced density matrix*.

whence the evolution of the one-qubit effective pure states:

$$\begin{aligned} U_Z(t)\bar{S}_1^x U_Z^\dagger(t) &= \cos(\omega_1 t)\bar{S}_1^x + \sin(\omega_1 t)\bar{S}_1^y, \\ U_Z(t)\bar{S}_1^y U_Z^\dagger(t) &= -\sin(\omega_1 t)\bar{S}_1^x + \cos(\omega_1 t)\bar{S}_1^y, \\ U_Z(t)\bar{S}_1^z U_Z^\dagger(t) &= \bar{S}_1^z. \end{aligned} \quad (181)$$

The Zeeman propagator $U_Z(t)$ rotates the spin around the z -axis an angle $\varphi := \omega_1 t$. It is customary to use the spectroscopist notation to denote the unitary action of the RF pulses in the rotating frame or interaction picture:

$$[\varphi]_i^\alpha := e^{-i\varphi\bar{S}_i^\alpha}, \quad \alpha = x, y, \quad i = 1, 2, \dots, n, \quad (182)$$

where φ is the rotation angle, α is the rotation axis, and i the index labelling the rotating qubit. Thus, the effect of a $[\pi]_1^x$ pulse

$$[\pi]_1^x = e^{-i\pi\bar{S}_1^x} = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \quad (183)$$

is,

$$\bar{S}_1^z \xrightarrow{[\pi]_1^x} -\bar{S}_1^z \quad \text{i.e. } |0\rangle\langle 0| \leftrightarrow |1\rangle\langle 1|. \quad (184)$$

Therefore, with a $[\pi]_1^x$ pulse effected on a non-interacting ensemble of single spins in thermal equilibrium, we can effectively simulate the quantum transition between the qubit states $|0\rangle$ and $|1\rangle$. In the thermal equilibrium ensemble, there is an excess of populated ground states with respect to the populations of excited states. After applying the pulse, the populations are reversed. Likewise, a $[\frac{1}{2}\pi]_1^x$ pulse produces off-diagonal terms in the density matrix at finite temperature that simulates quantum superpositions of pure states.

For multiqubit states, the correspondence between pure states and spin density matrices is not so simple. Let us consider the case of two-qubit states. It is possible to extend the description of multi-spin density matrix using the so-called *product operator formalism* by the NMR spectroscopists. Thus, the density matrix for the pure ground state $|\Psi\rangle = |00\rangle$ is

$$\rho_{|\Psi\rangle} := |00\rangle\langle 00| = \frac{1}{2}(\frac{1}{2} + \bar{S}_1^z + \bar{S}_2^z + 2\bar{S}_1^z\bar{S}_2^z). \quad (185)$$

In general, any density matrix can be expanded in a tensor product basis of one-spin operators $\{\bar{S}_i^x, \bar{S}_i^y, \bar{S}_i^z\}_{i=1, \dots, n}$. For n qubits,

$$\begin{aligned} \rho &= \sum_{\alpha_1, \dots, \alpha_n} c_{\alpha_1, \dots, \alpha_n} \sigma_1^{\alpha_1} \dots \sigma_n^{\alpha_n}, \\ c_{\alpha_1, \dots, \alpha_n} &:= 2^{-n} \text{Tr}(\rho \sigma_1^{\alpha_1} \dots \sigma_n^{\alpha_n}), \end{aligned} \quad (186)$$

where $\alpha_i = 0, x, y, z$, and $\sigma_i^0 := 1$.

This has the advantage that the evolution of the ensemble density matrix is then simply determined through the evolution rules for single spin operators. The problem that we face now is that the thermal equilibrium

matrix in the high-temperature limit $k_B T \gg \hbar\omega_i$ for the Hamiltonian (172) is

$$\rho_2 = \frac{1}{4} - \frac{1}{8}\hbar\beta \text{diag}(\omega_1 + \omega_2 + J_{12}, \omega_1 - \omega_2 - J_{12}, -\omega_1 + \omega_2 - J_{12}, -\omega_1 - \omega_2 + J_{12}), \quad (187)$$

which is further approximated assuming a weak coupling regime $|\omega_1 - \omega_2|, |J_{1,2}| \ll |\omega_1 + \omega_2|/2$ to

$$\rho_2 \simeq \frac{1}{4} - \epsilon_2(\bar{S}_1^z + \bar{S}_2^z), \quad \epsilon_2 := \frac{1}{8}\hbar(\omega_1 + \omega_2)/k_B T, \quad (188)$$

and the corresponding deviation matrix $\delta_2 := \bar{S}_1^z + \bar{S}_2^z$ is not equivalent to the initial quantum ground state (185) we want to simulate. This is the *initialization problem* in NMR computing.

4. Logic gates with NMR

To prepare the ensemble of spins in the referential state (185) as well as to implement the logical operations for quantum processing, we need to resort to a series of well-known techniques in NMR liquid spectroscopy to carry out controlled time evolution of spins:

i) *Rabi pulses*. The associated external Hamiltonian (171) corresponds to a harmonically oscillating magnetic field perpendicular to the Zeeman axis. It is applied at resonance and its effect on a single spin in the z -direction is the following

$$\begin{aligned} [\varphi]_1^x : S_1^z &\mapsto \cos(\varphi)S_1^z - \sin(\varphi)S_1^y, \\ [\varphi]_1^y : S_1^z &\mapsto \cos(\varphi)S_1^z + \sin(\varphi)S_1^x, \end{aligned} \quad (189)$$

where $\varphi := \Omega t$, t being the time duration and Ω the Rabi frequency.

ii) *Chemical-shift pulses*. They act as the propagator generated by the Zeeman part of the internal Hamiltonian (171). Their effect on the spin operators is given by (181).

iii) *Scalar pulses*. These induce the time evolution under the scalar coupling (two-spin) part of the internal Hamiltonian (171). For two qubits labelled 1,2, this scalar coupling propagator is also diagonal in the computational basis:

$$U_J(t) = e^{-i2J_{12}t\bar{S}_1^z\bar{S}_2^z} = \cos(\frac{1}{2}J_{12}t) - 4i\sin(\frac{1}{2}J_{12}t)\bar{S}_1^z\bar{S}_2^z, \quad (190)$$

and its effect on single spin operators is

$$\begin{aligned} U_J(t)\bar{S}_1^x U_J^\dagger(t) &= \cos(J_{12}t)\bar{S}_1^x + 2\sin(J_{12}t)\bar{S}_1^y\bar{S}_2^z, \\ U_J(t)\bar{S}_1^y U_J^\dagger(t) &= \cos(J_{12}t)\bar{S}_1^y - 2\sin(J_{12}t)\bar{S}_1^x\bar{S}_2^z, \\ U_J(t)\bar{S}_1^z U_J^\dagger(t) &= \bar{S}_1^z. \end{aligned} \quad (191)$$

The NMR spectroscopist notation for these pulses is

$$[\varphi]_{12}^J := e^{-i2J_{12}t\bar{S}_1^z\bar{S}_2^z}, \quad (192)$$

where the rotation angle is $\varphi = J_{12}t$ and the subscript denotes the spins involved in the scalar pulse.

iv) *Gradient pulses.* This is the technique used in the spatial averaging formalism of Cory et al. (1996; 1997). It consists in applying an external Hamiltonian (171) in the form of a field gradient along the liquid sample:

$$H_{\text{grad}} = - \sum_{i=1}^n \gamma_i (z \partial_z B^z)_{z=z_i} S_i^z, \quad (193)$$

where z_i is the coordinate of the i -th spin in the sample along the direction of the applied field gradient. This produces a spatially varying distribution of states throughout the sample. Its effect is to create a position-dependent phase shift with zero average, causing the vanishing of non-diagonal elements of the density matrix. The notation for these pulses is $[\text{grad}]^z$.

This gradient method is used to selectively turn off the tranverse (x, y) spin factors in the product operator expansion of the density matrix, while leaving untouched the rest. For example, it is possible to induce the following transformation

$$[\text{grad}]^z : \bar{S}_1^z + \bar{S}_2^x \mapsto \bar{S}_1^z. \quad (194)$$

Now, the combined effect of the following series of pulses (Jones, 2000) produces the reference state (185) starting from the thermal ensemble of spins (188):⁷¹

$$\begin{aligned} & \bar{S}_1^z + \bar{S}_2^z \\ & \xrightarrow{[\pi/3]_2^z} \bar{S}_1^z + \frac{1}{2}\bar{S}_2^z - \frac{\sqrt{3}}{2}\bar{S}_2^y \\ & \xrightarrow{[\text{grad}]^z} \bar{S}_1^z + \frac{1}{2}\bar{S}_2^z \\ & \xrightarrow{[\pi/4]_1^x} \frac{1}{\sqrt{2}}\bar{S}_1^z - \frac{1}{\sqrt{2}}\bar{S}_1^y + \frac{1}{2}\bar{S}_2^z \\ & \xrightarrow{[\pi/2]_{12}^J} \frac{1}{\sqrt{2}}\bar{S}_1^z + \frac{1}{\sqrt{2}}2\bar{S}_1^x\bar{S}_2^z + \frac{1}{2}\bar{S}_2^z \\ & \xrightarrow{[-\pi/4]_1^y} \frac{1}{2}\bar{S}_1^z - \frac{1}{2}\bar{S}_1^x + \frac{1}{2}2\bar{S}_1^x\bar{S}_2^z + \frac{1}{2}\bar{S}_2^z + \frac{1}{2}2\bar{S}_1^z\bar{S}_2^z \\ & \xrightarrow{[\text{grad}]^z} \frac{1}{2}\bar{S}_1^z + \frac{1}{2}\bar{S}_2^z + \frac{1}{2}2\bar{S}_1^z\bar{S}_2^z. \end{aligned} \quad (195)$$

Once we have the reference state available, we can proceed to effectively simulate other quantum states applying series of pulses to produce the desired ensemble of spin states. For instance, the density matrix of the Bell state $|\Psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ in the product operator formalism is

$$\rho_{|\Psi\rangle} = \frac{1}{2} \left(\frac{1}{2} + 2\bar{S}_1^z\bar{S}_2^z + 2\bar{S}_1^x\bar{S}_2^x - 2\bar{S}_1^y\bar{S}_2^y \right), \quad (196)$$

which can be reached from the ground state $|00\rangle$ with the unitary operator

$$U = e^{-i\pi\bar{S}_1^x\bar{S}_2^y}. \quad (197)$$

This propagator, in turn, can be simulated with the following series of NMR pulses (from right to left):

$$[\frac{1}{2}\pi]_2^x [-\frac{1}{2}\pi]_1^y [\frac{1}{2}\pi]_{12}^J [\frac{1}{2}\pi]_1^y [-\frac{1}{2}\pi]_2^x : \rho_{|00\rangle} \mapsto \rho_{|\Psi\rangle}. \quad (198)$$

Likewise, the controlled-NOT gate is simulated by the following sequence:

$$[-\frac{1}{2}\pi]_2^y [-\frac{1}{2}\pi]_2^z [\frac{1}{2}\pi]_1^z [\frac{1}{2}\pi]_{12}^J [\frac{1}{2}\pi]_2^y. \quad (199)$$

In a similar fashion, one can implement other quantum states and logic gates. Actually, this NMR pulse technique has been so highly developed that it is possible to simulate the propagator of a set of interacting spins with any desired couplings, even turning on and off certain spin couplings at will. For this reason, this capability for controlling the NMR dynamics is referred to as *spin choreography* (Freeman, 1998).

The logical labelling formalism of Gershenfeld and Chuang (1997) uses a different strategy to prepare pseudo-pure states. It is based in the appropriate embedding of a set of spin states into a larger system. It does not resort to field gradients but instead these auxiliary spin states are used to implement the quantum computation with several qubits. There are also experimental realizations of this scheme (Vandersypen et al., 1999).

5. Measurements

Once the NMR computation is over, we have to read out the result from the spectrometer. This is done by measuring the macroscopic magnetization of the liquid sample with a detection coil (see Fig. 50). This bulk magnetization induces currents in the transverse RF coil which is tuned to the resonance frequency. The RF coil generates a dipole field and only the dipolar components of the density matrix oriented along the transversal magnetic field will couple to the measurement device.

In computing with NMR ensembles, measuring an observable (176) entails a perturbation softer than for pure states, where measurement is a strong projective process. The measured currents are proportional to the following trace (Cory et al., 2000)

$$\text{Tr} \left(\sum_{i=1}^n \bar{S}_i^+ \rho \right), \quad (200)$$

with $\bar{S}_i^+ := \bar{S}_i^x + i\bar{S}_i^y$. For instance, the signal (200) due to the precession induced on $\bar{S}_i^x, i = 1, 2$, by the chemical-shifts and scalar-coupling pulses acting on a two-qubit molecule such as the 2,3-dibromo-thiophene (Fig. 49 a)), is shown in Fig. 51. This is the Fourier-transformed real part of the signal (Cory, Price and Havel, 1997) and clearly shows the populations peaks corresponding to the 4 states of a two-spin system depicted in Fig. 43. This is called an *in-phase doublet* for both peaks have the same sign. For different series of pulses the pattern of the signal changes accordingly and this allows to retrieve the

⁷¹This sequence is not necessarily unique.

information contained in the ensemble of states. When implementing simple quantum algorithms with NMR liquid spectroscopy, the output retrieval is performed by analysing a subset of resonances, but in more general situations a technique called *quantum state tomography* is used to systematically obtain the final quantum state (Knill, Chuang and Laflamme, 1997).

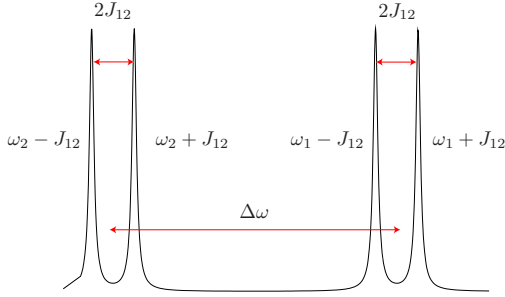


FIG. 51: Schematic signal from a NMR liquid spectrometer corresponding to an in-phase doublet for a two-spin system with energy levels as in Fig. 43. Notice that here the frequencies are positive.

6. Achievements and limitations

There is an extensive list of experimental achievements in NMR quantum computing (Cory et al., 2000). Just to quote a few of them, two-qubit gates have been constructed by several groups (Cory, Fahmy and Havel, 1996; Chuang et al., 1997; Collins et al., 1999), the Toffoli gate has also been implemented (Price et al., 1999), as well as the quantum Fourier transform (Weinstein, Lloyd, and Cory, 1999), quantum teleportation (Nielsen, Knill and Laflamme, 1998), etc., and there are NMR experiments involving 7-qubits (Knill et al., 2000). An alternative approach to implement NMR quantum computation uses geometric phase-shift gates (Jones et al., 2000) where the controlled phases are Berry phases.

Despite the list of successes in NMR quantum computing, there are currently strong limitations in the scalability of the pseudo-pure state preparation: it is clear from (174) that the deviation density matrix used in high-temperature NMR scales exponentially down with the factor 2^{-n} . This is a severe limitation that reduces the ratio of the observable signal to the background noise. To overcome this inefficiency we would need an exponentially large system.⁷² It is currently estimated that it is not possible to go well beyond 10 qubits using NMR

liquid state methods. This and other shortcomings has led to pursue other NMR-like proposals, but this time based on solid state samples (Cory et al., 2000), with the aim at using true pure states. The goals set for these proposals are to reach 10-30 qubits, still not far enough for competitive purposes.

The use of mixed states in NMR computing and the fact that they are exponentially inefficient have raised doubts about the truly quantum nature of the computations carried out by NMR liquid spectroscopy. The main objection comes from the result by Braunstein et al. (1999) showing that all the pseudo-pure states used so far in NMR are separable, with no entanglement. This does not invalidate the exponential speed-up obtained with the implementation of quantum algorithms.⁷³

C. Solid-State Quantum Computers

There are several proposals for building a quantum computer with some sort of solid-state device. We have just mentioned that a possible cure for the shortcomings of bulk NMR liquid computation is precisely resorting to solid NMR techniques. One type of proposals uses macroscopic superconducting devices with a radio frequency SQUID as the qubit (Averin, 1998). The presence of 0 or 1 quanta of flux is the two-state system. Several ways to couple the SQUIDS to make logic circuits exist, like using Josephson tunnel junctions (Makhlin, Schön and Shnirman, 2001). Other type of designs rely on quantum dot nanotechnology: Barenco et al. (1995) proposed using both charge and spin degrees of freedom for qubits in quantum dots, addressed respectively with electric and magnetic fields. Loss and DiVincenzo (1998) also propose using spin states of electrons in quantum dots as qubits.

The list of experimental proposals is too large by now to be covered in detail. Instead, we shall focus on one of the most original proposals for doing solid-state quantum computation: this is Kane's idea (1998) for building a silicon-based quantum computer. This is an appealing program for Kane envisages the possibility of using the semiconductors used in most conventional computer electronics for building also a quantum computer, although the challenges to achieve this goal are still enormous. The belief though is that the silicon technology is a very rapidly developing field and there are chances to overcome those challenges.

The quantum hardware in Kane's proposal is an array of nuclear spins located on donors in silicon. Then, a qubit is the individual nuclear spin of Phosphor ^{31}P atoms; a quantum register is the whole array of ^{31}P

⁷²Something that happens in classical DNA computing (Adleman, 1994), where there is a trade-off between exponential computing time for solving a problem and exponential space for molecular states.

⁷³Whether working with separable states in NMR spectroscopy is a truly quantum computation or not is still a controversial issue (Jones, 2000).

dopants in Silicon ^{28}Si ; operations are effected using a combination of magnetic resonance techniques (Rabi pulses) with static electric fields; information is exchanged between nearby ^{31}P nuclear spins by means of the surrounding electrons.

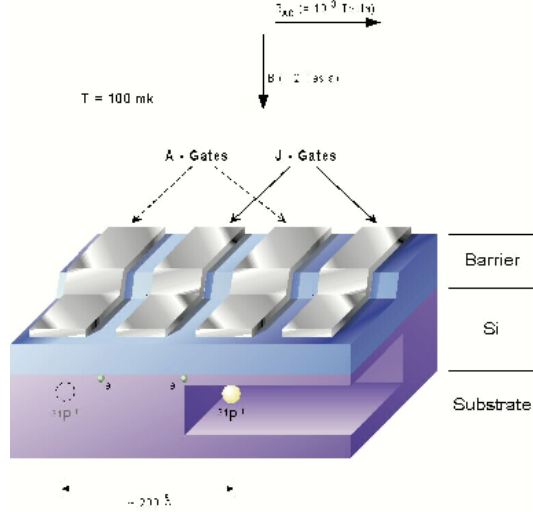


FIG. 52: Schematic design of a silicon-based quantum computer pursued by the group of South Wales university.

1. Semiconductors for quantum computation

The choice of nuclear spins in this case is again motivated by their extremely well isolation from the environment, like in the NMR proposal. A further requirement now is that the dopant spins must not interact appreciably with the spins of the host semiconductor. To guarantee this we demand that the chemical elements of the host have zero nuclear spin $S = 0$, to avoid undesired spin couplings. This singles out the semiconductor group V as a host candidate and removes other groups like III (with Ga) and IV (with As). Silicon ^{28}Si is an example of stable isotope in group V.

Unlike the NMR liquid spectroscopy, Kane's QC is neither a bulk spin quantum computation nor resorts to macroscopic magnetization measurements. Instead, it truly needs addressing spins individually for initialization and readout, and this is precisely one of the open challenges.

The basic ingredient in Kane's proposal is to trade direct nuclear spin interactions by electronic detections, which are likely to be easier to handle. Thus, the spin state of an individual nucleus dopant on a semiconductor will not be detected directly, but through its hyperfine interaction with the surrounding electrons. The hyperfine interaction is proportional to the probability density of the electrons at the nucleus. The electronic cloud is

sensitive to electric voltages and can in principle be externally manipulated. Moreover, in certain cases the electronic wave functions extend far enough so as to overlap with a neighbouring atom, thereby producing an indirect coupling between nuclear spins mediated by the atomic electrons. This indirect electron coupling can also be enhanced by applying external electric fields.

These conditions are met by shallow level donors like ^{31}P , for which the range of the electron wave function is of order 10-100 Å. In addition, within the group V, the only shallow donor in Si with nuclear spin $S = \frac{1}{2}$ is precisely ^{31}P . Therefore, the $^{31}\text{P}:\text{Si}$ system is a good candidate for a silicon based quantum computer. For instance, at low ^{31}P concentrations and low temperature $T = 1.5$ K, the electron spin relaxation time is order 10^3 s, and the nuclear spin relaxation time is over 10 hours. If the temperature is further reduced to $T \sim \text{mK}$, the phonon limited ^{31}P relaxation time is likely of the order of 10^{18} s (Kane, 1998).

2. External control fields

We see that in Kane's idea the electrons play a role similar to phonons in the Cirac-Zoller gate: they both mediate the conditional interactions between the real qubits. Likewise, we also need external electric fields to bring dopant nuclei close enough to interact. In all, we need to control three types of external fields:

1) Electric gates above the donors to control individual electronic states (see Fig. 52).

2) Electric gates between the donors to control interactions between qubits.

3) Constant B and oscillating B_{ac} magnetic fields to execute operations on the individual spins much akin to those we have described for nuclear spin resonance.

The scenario for replacing a Si vacancy by a P dopant atom is possible because both elements have similar sizes. Of the five outer (3p) electrons in a ^{31}P atom (one more than in Si), four of them will form covalent bonds with neighbouring Si atoms, while the remaining fifth electron is loosely bound to the ^{31}P atom. This outer electron and the rest of the dopant atom behave in first approximation as a Hydrogen-like atom embedded into a Si environment. At low temperatures, the electron state is 1s and this yields a large hyperfine interaction. The effective Bohr radius is estimated at 30 Å. To proceed with the quantum computation we need this electron to remain in its ground state, and to apply an external constant magnetic field to break the spin degeneracy. These conditions are met if $2\mu_B B \gg k_B T$, as for the typical values $B \geq 2$ T and $T \leq 100$ mK.

3. Logic gates

The description of the basic gate operations is the following:

i) *One-qubit A-gate.* The terminology is due to the A coupling constant of the hyperfine interaction between nuclear and electron spins. Single spin control is achieved by externally changing the voltage on a gate electrode (A -gate) located on top of each nucleus (see Fig. 52); spin-flips are then driven by a Rabi pulse tuned to the resonance frequency for the particular spin.

The one-qubit Hamiltonian H_1 modelling the interaction between the nuclear spin (denoted by n) and the electronic spin (denoted by e) in the presence of a constant magnetic field B is

$$\begin{aligned} H_1 &:= H_{1,Z} + (A/\hbar^2) \mathbf{S}_{n,1} \cdot \mathbf{S}_{e,1}, \\ H_{1,Z} &:= -\gamma_n S_{n,1}^z B - \gamma_e S_{e,1}^z B, \end{aligned} \quad (201)$$

where $\mathbf{S}_{n,1}$, $\mathbf{S}_{e,1}$ are the nuclear and electron spins, $\gamma_n \mathbf{S}_{n,1}$, $\gamma_e \mathbf{S}_{e,1}$ their corresponding magnetic moments, and

$$A := -\frac{8\pi}{3} \bar{\gamma}_n \bar{\gamma}_e |\Psi(0)|^2, \text{ with } \bar{\gamma}_n := \hbar \gamma_n, \bar{\gamma}_e := \hbar \gamma_e, \quad (202)$$

is the contact hyperfine interaction energy, with $|\Psi(0)|^2$ the probability density of the electron wave function at the nucleus position. Note that $\bar{\gamma}_e = -g_e \mu_B$, $\bar{\gamma}_n = g_n \mu_N$, where $g_e = 2$, $g_n \approx 2 \times 1.13$ are, respectively, the relevant electron Landé g -factor and the nuclear gyromagnetic factor in $^{31}\text{P}:\text{Si}$. Under operating conditions the electron remains in its ground state, and the separation of the nuclear spin levels is, to second order in the hyperfine coupling $A \ll \bar{\gamma}_n B$:⁷⁴

$$\hbar \omega_A = \bar{\gamma}_n B + \frac{A}{2} - \frac{A^2}{4\bar{\gamma}_e B}. \quad (203)$$

In $^{31}\text{P}:\text{Si}$, $A/2\hbar = 58$ MHz and therefore $A > \bar{\gamma}_n B$ for $B < 3.5$ T. We can have control over this energy gap with the static electric field applied with the A -gate (see Fig. 52). This shifts the electron wave function away from the nucleus (see Fig. 53) and reduces the hyperfine interaction A in (202). Thus, the frequency (203) of the nuclear spins is controlled externally and this allows us to bring them into resonance with the oscillating pulse B_{ac} in order to effect arbitrary one-spin rotations.

ii) *Two-qubit J -gate.* The name is suggested by the J spin-exchange coupling between electron spins. Conditional logic operations are possible because of electron-mediated interactions between the nuclear spins of two Kane's qubits when brought sufficiently close by an externally applied voltage (J) gate (see Fig. 52). The two-qubit Hamiltonian is then

$$H_{12} = \sum_{i=1}^2 (H_{i,Z} + A_i \bar{\mathbf{S}}_i^n \cdot \bar{\mathbf{S}}_i^e) + J \bar{\mathbf{S}}_1^e \cdot \bar{\mathbf{S}}_2^e, \quad (204)$$

⁷⁴We have also approximated $-\gamma_e B + \gamma_n B$ by $-\gamma_e B$ in the denominator of (203).

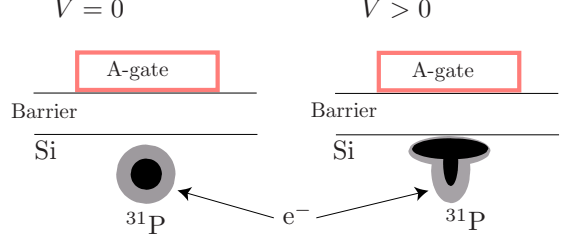


FIG. 53: Pictorial representation of an A -gate that controls the nucleus-electron system (201). An externally applied electric field shifts the electron wavefunction from the donor ^{31}P , reducing the contact hyperfine interaction (202).

where $H_{i,Z}$ are the Zeeman Hamiltonians for each qubit (201), A_i are the hyperfine couplings for each nucleus-electron system and J is the exchange coupling interaction between electron spins. This exchange energy depends on the overlap of the electron wave functions. Treating the ^{31}P dopants as Hydrogen-like atoms in first approximation, the J coupling can be estimated for well separated donors as (Herring and Flicker, 1964)

$$J(r) \simeq 1.6 \frac{e^2}{\epsilon a_B} \left(\frac{r}{a_B} \right)^{5/2} e^{-2r/a_B} \quad (205)$$

with r the inter-donor distance, $\epsilon = 11.7$ the Si dielectric constant and a_B the Bohr radius of the atom. As the J coupling depends on the electron overlapping, we can use again a voltage gate between the donors to distort the electron clouds in order to control their coupling strength (see Fig. 54). This coupling will be significant when $J \simeq |\bar{\gamma}_e|B/2$ and this corresponds to a donor separation of order 100-200 Å (Kane, 1998), which is not far from the current limits of atom-scale lithography.

The relevant energy levels for doing quantum computation with a two-qubit Hamiltonian (204) are easily found (Berman et al., 1999). This Hamiltonian is a 16×16 matrix. We shall label the basis states with the components of the nuclear and electron spins at each donor site, with $|0\rangle_n, |1\rangle_n$ denoting nuclear spins (up and down) and $|\uparrow\rangle_e, |\downarrow\rangle_e$ for the electron spins; for instance,

$$|11\rangle_n |\downarrow\downarrow\rangle_e \quad (206)$$

represents a state with both nuclear and electron spins down.

In the presence of a static magnetic field and for low temperatures ($k_B T \ll |\bar{\gamma}_e|B$), the electrons remain with the spins down polarized $|\downarrow\downarrow\rangle_e$. For example, $B = 2$ T, $T = 100$ mK meet this requirement. However, we shall see that switching the J -gate on may change such state, which will be the basis for doing spin measurements.

The essence of the functioning of the J -gate is to enhance the overlap between the electron wave functions of two nearest ^{31}P donors. In this way, the

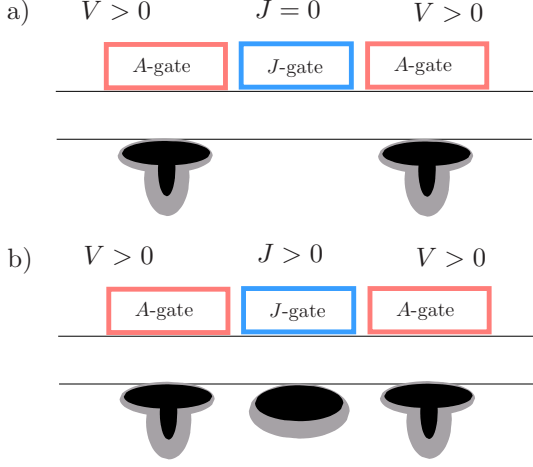


FIG. 54: Pictorial representation of a J -gate that controls the nucleus-electron-nucleus system (204). When the electrostatic potential of the J -gate is off (a)) or on (b)), the J -exchange coupling in (204) gets reduced or enhanced, respectively.

^{31}P nuclear spins (Kane qubits) can be indirectly coupled one another through the electron mediated interaction J . To perform two-qubit quantum logic gates, we need to address individually the 4 nuclear spin states $\{|00\rangle_n, |01\rangle_n, |10\rangle_n, |11\rangle_n\}$. For simplicity, we assume $A_1 = A_2 = A$. In the absence of J -coupling the states $|01\rangle_n |\downarrow\downarrow\rangle_e, |10\rangle_n |\downarrow\downarrow\rangle_e$ are degenerate. These states belong to the sector of total z -component of spin $\bar{S}_{\text{tot}}^z := (\bar{S}_{1,n}^z + \bar{S}_{2,n}^z) + (\bar{S}_{1,e}^z + \bar{S}_{2,e}^z) = -1$. The role of the J -gate is precisely to control this energy splitting, which we now try to estimate.

Let us consider the Kane implementation of the CNOT-gate (Goan and Milburn, 2000). There are four steps involved:

1/ We start with $J = A_2 - A_1 = 0$, so that the states $\{|00\rangle_n |\downarrow\downarrow\rangle_e, |01\rangle_n |\downarrow\downarrow\rangle_e, |10\rangle_n |\downarrow\downarrow\rangle_e, |11\rangle_n |\downarrow\downarrow\rangle_e\}$ have energies

$$\begin{aligned} E_{|00\rangle_n |\downarrow\downarrow\rangle_e} &= -\sqrt{(-\bar{\gamma}_e + \bar{\gamma}_n)^2 B^2 + A^2} - \frac{1}{2}A, \\ E_{|01\rangle_n |\downarrow\downarrow\rangle_e} &= E_{|10\rangle_n |\downarrow\downarrow\rangle_e} = \\ &= \frac{1}{2}((\bar{\gamma}_e + \bar{\gamma}_n)B - \sqrt{(-\bar{\gamma}_e + \bar{\gamma}_n)^2 B^2 + A^2}), \\ E_{|11\rangle_n |\downarrow\downarrow\rangle_e} &= (\bar{\gamma}_e - \bar{\gamma}_n)B + \frac{1}{2}A. \end{aligned} \quad (207)$$

2/ Next one introduces a bias between the two A -gates by adiabatically switching on a difference $\Delta A := A_1 - A_2$ in their couplings, while keeping still $J = 0$. This splits the degeneracy of the $|01\rangle_n |\downarrow\downarrow\rangle_e, |10\rangle_n |\downarrow\downarrow\rangle_e$ states, allowing us to choose one as a control qubit and the other

as a target qubit. The energies in (207) become

$$\begin{aligned} E_{|00\rangle_n |\downarrow\downarrow\rangle_e} &= -\frac{1}{2}(\sqrt{(-\bar{\gamma}_e + \bar{\gamma}_n)^2 B^2 + A_1^2} \\ &+ \sqrt{(-\bar{\gamma}_e + \bar{\gamma}_n)^2 B^2 + A_2^2}) - \frac{1}{4}(A_1 + A_2), \\ E_{|01\rangle_n |\downarrow\downarrow\rangle_e} &= -\frac{1}{4}\Delta A \\ &+ \frac{1}{2}((\bar{\gamma}_e + \bar{\gamma}_n)B - \sqrt{(-\bar{\gamma}_e + \bar{\gamma}_n)^2 B^2 + A_1^2}), \\ E_{|10\rangle_n |\downarrow\downarrow\rangle_e} &= \frac{1}{4}\Delta A \\ &+ \frac{1}{2}((\bar{\gamma}_e + \bar{\gamma}_n)B - \sqrt{(-\bar{\gamma}_e + \bar{\gamma}_n)^2 B^2 + A_2^2}), \\ E_{|11\rangle_n |\downarrow\downarrow\rangle_e} &= (\bar{\gamma}_e - \bar{\gamma}_n)B + \frac{1}{4}(A_1 + A_2), \end{aligned} \quad (208)$$

and the corresponding eigenstates are still $\{|00\rangle_n |\downarrow\downarrow\rangle_e, |01\rangle_n |\downarrow\downarrow\rangle_e, |10\rangle_n |\downarrow\downarrow\rangle_e, |11\rangle_n |\downarrow\downarrow\rangle_e\}$, predominantly.

3/ Once the two qubits are distinguished energetically it is time to introduce, again adiabatically, the J -coupling to bring the states $|10\rangle_n$ and $|01\rangle_n$ to the symmetric and antisymmetric combinations, namely

$$\begin{aligned} |10\rangle_n &\mapsto |s\rangle_n := 2^{-1/2}(|01\rangle_n + |10\rangle_n), \\ |01\rangle_n &\mapsto |a\rangle_n := 2^{-1/2}(|01\rangle_n - |10\rangle_n). \end{aligned} \quad (209)$$

For this purpose it is necessary to keep J at full strength before switching off adiabatically ΔA .

The energies of the new eigenstates both in presence of A - and J -couplings, with $\Delta A = 0$, can be computed exactly by diagonalizing H_{12} in the sectors of fixed total 3th component S_{tot}^z of the spin, since this is a conserved quantity. Only the values $S_{\text{tot}}^z = -2, -1, 0$ are relevant for our discussion, since our initial states lie there. First we need to know the energy splitting $\hbar\omega_J$ between the symmetric and antisymmetric qubit states in the sector $S_{\text{tot}}^z = -1$. Second, to control the Rabi pulse in the coming step, the gap energy $\hbar\omega_{\text{ac}}$ between $|s\rangle_n |\downarrow\downarrow\rangle_e$ and $|11\rangle_n |\downarrow\downarrow\rangle_e$ must also be known.

To calculate $\hbar\omega_J$ we use the reduced basis

$$\{|01\rangle_n |\downarrow\downarrow\rangle_e, |10\rangle_n |\downarrow\downarrow\rangle_e, |11\rangle_n |\downarrow\uparrow\rangle_e, |11\rangle_n |\uparrow\downarrow\rangle_e\} \quad (210)$$

to express the Hamiltonian H_{12} in the sector $S_{\text{tot}}^z = -1$ as the following matrix

$$H_{(-1)} = \begin{pmatrix} \frac{1}{4}J + \bar{\gamma}_e B & 0 & 0 & \frac{1}{2}A \\ 0 & \frac{1}{4}J + \bar{\gamma}_e B & \frac{1}{2}A & 0 \\ 0 & \frac{1}{2}A & -\frac{1}{4}J + \bar{\gamma}_n B & \frac{1}{2}J \\ \frac{1}{2}A & 0 & \frac{1}{2}J & -\frac{1}{4}J + \bar{\gamma}_n B \end{pmatrix}. \quad (211)$$

As $A_1 = A_2 = A$, the two-qubit Hamiltonian is symmetric under the site labels and its eigenvectors can either be symmetric or antisymmetric under this exchange. The two symmetric (unnormalized) eigenstates are given by

$$\begin{aligned} |s, \pm\rangle &:= \\ &(\bar{\gamma}_n B + \frac{1}{4}J - E_{s,\pm})|s\rangle_n |\downarrow\downarrow\rangle_e + \frac{1}{2}A|00\rangle_n |s\rangle_e, \end{aligned} \quad (212)$$

where

$$\begin{aligned} |s\rangle_e &:= \frac{1}{\sqrt{2}}(|\downarrow\downarrow\rangle_e + |\uparrow\uparrow\rangle_e), \\ E_{s,\pm} &:= \frac{1}{2}(\bar{\gamma}_e + \bar{\gamma}_n)B + \frac{1}{4}J \pm \frac{1}{2}\sqrt{(-\bar{\gamma}_e + \bar{\gamma}_n)^2 B^2 + A^2}. \end{aligned} \quad (213)$$

Similarly the two antisymmetric (unnormalized) eigenstates are

$$\begin{aligned} |a, \pm\rangle &:= \\ &-(-\bar{\gamma}_e B - \frac{1}{4}J + E_{a,\pm})|00\rangle_n |a\rangle_e - \frac{1}{2}A|a\rangle_n |\downarrow\downarrow\rangle_e, \end{aligned} \quad (214)$$

with

$$\begin{aligned} |a\rangle_e &:= \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle_e - |\uparrow\downarrow\rangle_e), \\ E_{a,\pm} &:= \frac{1}{2}(\bar{\gamma}_e + \bar{\gamma}_n)B - \frac{1}{4}J \\ &\pm \frac{1}{2}\sqrt{((-\bar{\gamma}_e + \bar{\gamma}_n)B - J)^2 + A^2}. \end{aligned} \quad (215)$$

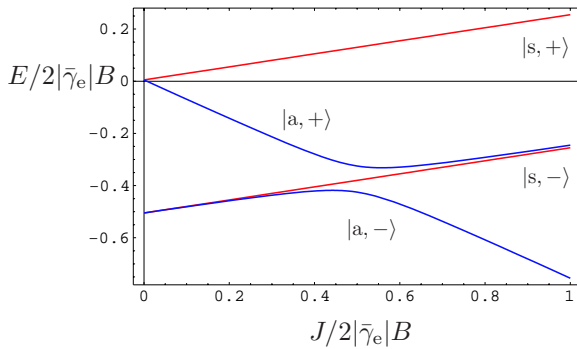


FIG. 55: Energy levels for a two-donor interacting system as a function of the exchange coupling J , for $A = 0.2|\bar{\gamma}_e|B$.

In Fig. 55 the energies $E_{s,\pm}, E_{a,\pm}$ are plotted against the exchange coupling constant J . For a two-electron spin system with antiferromagnetic coupling ($J > 0$), the exchange interaction lowers the energy of the spin singlet with respect to the triplets. When the static magnetic field is applied, the electron ground state is $|\downarrow\downarrow\rangle_e$ for $J < |\bar{\gamma}_e|B$. The exchange coupling can be increased adiabatically by external manipulation of the J voltage gate. For $J > |\bar{\gamma}_e|B$, the electron ground state is the singlet. The value $J = |\bar{\gamma}_e|B$ corresponds to the case where levels $E_{a,+}$ and $E_{s,-}$ avoid their crossing (Fig. 55). The energy splitting to be controlled with the J -gate is $\hbar\omega_J := E_{s,-} - E_{a,-}$, which can be estimated using the exact formulas (213), (215) and treating the hyperfine interaction as a small perturbation (assuming $J < |\bar{\gamma}_e|B$):

$$\hbar\omega_J \simeq \frac{A^2}{4} \left(\frac{1}{|\bar{\gamma}_e|B - J} - \frac{1}{|\bar{\gamma}_e|B} \right) \quad (216)$$

For the $^{31}\text{P}:\text{Si}$ system at $B = 2$ T and $J/h = 30$ GHz, (216) gives $\nu_J = 75$ kHz as the nuclear spin exchange

frequency. This is roughly the rate at which binary operations can be performed in the purported quantum computer. Recall that the speed for individual spin operations is determined by the oscillating field B_{ac} , and this speed is comparable to 75 kHz when $B_{ac} \sim 10^{-3}$ T.

To calculate finally the gap $\hbar\omega_{ac}$, we just need the energy of the state $|11\rangle_n |\downarrow\downarrow\rangle_e$ which lies in the trivial sector $S_{\text{tot}}^z = -2$:

$$E_{|11\rangle_n |\downarrow\downarrow\rangle_e} = (\bar{\gamma}_e + \bar{\gamma}_n)B + \frac{1}{4}J + \frac{1}{2}A. \quad (217)$$

4/ The moment is right to enforce the CNOT operation. This amounts to swap the states $|s\rangle_n$ and $|11\rangle_n$, which are well separated in energies by previous steps, while leaving the two other states untouched. To this aim, it suffices now to apply a Rabi pulse $H_{ac}(t) := -\gamma_n(S_{n,1}^x + S_{n,2}^x)B_{ac} \sin \omega_{ac}t$ resonant with the separation energy between the states to be exchanged. Although the gaps $E_{|11\rangle_n |\downarrow\downarrow\rangle_e} - E_{|s\rangle_n |\downarrow\downarrow\rangle_e}$ and $E_{|a\rangle_n |\downarrow\downarrow\rangle_e} - E_{|00\rangle_n |\downarrow\downarrow\rangle_e}$ are very close one each other, however the spin part of the magnetic interaction $H_{ac}(t)$ only couples in first order the states $|s\rangle_n$ and $|11\rangle_n$ and thus it does not affect essentially the states $|a\rangle_n$ and $|00\rangle_n$. To complete the CNOT-gate one applies backwards the steps 3/, 2/ and 1/ (see Fig. 56).

Other computer operations such as spin measurements and initialization of the quantum register are also based on the adiabatic manipulation of the A - and J -voltages. The underlying idea has been to correlate nuclear spin states adiabatically with states of electron spins, which in turn affect the symmetry of the electron orbital wave function (Kane, 2000).

Unlike the QC proposals based on ion-traps or NMR spectroscopy, the silicon-based QC has not been yet implemented experimentally.⁷⁵ This will require nanofabrication at the atomic scale involving at least specialized techniques such as quantum electronic measurements with Single Electron Transistors (SET) for addressing individual qubits, atom-scale lithography to place Phosphorus donors in a Silicon crystal with near-atomic precision, combined with electron beam lithography for building the quantum array of qubits, etc. (Kane, 2000). It remains an open issue whether the current developments in these technologies will be enough to build a Kane quantum computer.

XII. CONCLUSIONS

Although this may look an extensive review, the field has grown at such a pace that it is not possible to cover in detail all the interesting developments going on, and

⁷⁵There is a funded project in the Semiconductor Nanofabrication Facility of the South Wales University (Australia) for building a Kane's quantum computer.

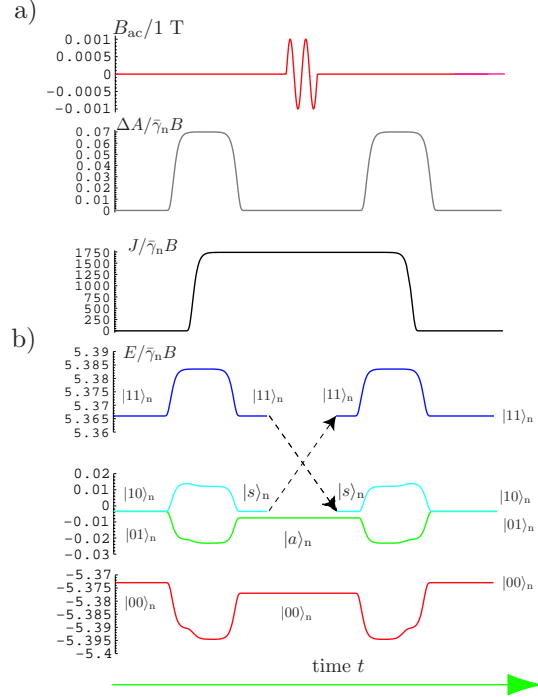


FIG. 56: Implementation of the CNOT-gate in a Kane quantum computer as described in steps 1/-4/ in text (time t runs along the horizontal axis). In a) the externally driven couplings are shown, and in b) the qubits energies are plotted, conveniently shifted by $E \mapsto E - \bar{\gamma}_e B - \frac{1}{4}J$.

many have been left out. Just to mention a few of them: universal sets of fault-tolerant quantum gates, a thorough study of decoherence problems, quantum erasure, further experimental proposals for quantum computers, etc.

We share the belief in the mutual benefit of the symbiosis between quanta and information. The very knowledge of the foundations of physics can benefit from the theory of information and computation (Landauer, 1991; 1996). We have reviewed some of the aspects coming out from the fruitful idea that information is physics. We could further speculate all the way around: physics is also information. It might quite well be the case that a fundamental theory of physics could be based on the notion of qubit from which all the rest would be derived (Wheeler, 1990; Zeilinger, 1999).

We have made an effort to present both classical and quantum aspects of information and computation. Classical aspects have been traditionally linked to computer science, of interest both to computer and electronic engineers, and to mathematicians addressing its theoretical and abstract foundations. Quantum aspects, on the contrary, have been almost uniquely associated to quantum physicists. Thus, each community finds its own barrier in order to jump over and to enter the field of quantum computation: an engineer lacks frequently the necessary training in quantum theory while most physicists are

not used to deal with elementary aspects of information and the insides of a real computer. These shortcomings make traditionally difficult to bring together both type of researchers. Our work is aimed in part at setting up a bridge between both communities in the belief that it will be rewarding for both of them. We are confident that after this quantum information revolution time will be ripe for quantum mechanics to be taught regularly at engineer schools, and for information theory to figure among background courses in physics. Moreover, by presenting a brief account of the experimental realization of quantum computers we also stress the close relationship with other particular fields like condensed matter and its many branches, specially with the area of strongly correlated systems.

There is currently a big interest in building real quantum computers, capable of doing non-trivial tasks. Also, a bunch of new proposals have been presented and this trend is likely to continue. Each physical system or interaction in nature is scrutinized as a possible realization of a quantum computer. Marvelous machines, like aircrafts, were envisaged in the past by Leonardo da Vinci; he described them on a piece of paper and were not actually built up until hundreds of years later. Likewise, nowadays we find theoretical designs of prospective quantum computers. We hope that in the case of quantum computers this process will not take that long. At least for the current modest realizations the elapsed time has been short. Even these modest realizations are remarkable since they allow for testing some of the theoretical principles.

Now we come necessarily to an end. And we close with a grand query. We have talked about a large variety of computer machines: classical – both sequential and parallel machines of many types – and quantum mechanical – both theoretical and experimental. Yet, there is a marvellous machine which plays a paramount role in all those constructions, because after all, it is the one that has devised them all. And thus, it is also natural to ask: what type of computer machine is the human brain?

ACKNOWLEDGMENTS

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LIST OF SYMBOLS AND ACRONYMS

BB84: Bennett-Brassad 1984

B92: Bennett 1992
BBPSSW96: Bennett-Brassard-Popescu-Schumacher-Smolin-Wooters 1996
CPU: Central Processing Unit
E91: Ekert 1991
ECCC: Error-Correcting Classical Code
EDP: Entanglement Distillation Protocol
EPR: Einstein-Podolsky-Rosen
GNFS: General Number Field Sieve
LOCC: Local Operations Classical Communications
MIPS: Million Instructions Per Second
NDTM: Nondeterministic Turing Machine
NMR: Nuclear Magnetic Resonance
NP: Class of nondeterministic polynomial-time problems
P: Class of deterministic polynomial-time problems
PKC: Public Key Cryptography
PTM: Probabilistic Turing Machine
QC: Quantum Computer
QECC: Quantum Error Correction Code
QFT: Quantum Fourier Transform
QKD: Quantum Key Distribution
QTM: Quantum Turing Machine
RF: Radio Frequency
RSA: Rivest-Shamir-Adleman
TM: Turing Machine
VNM: Von Neumann Machine

APPENDIX: COMPUTATIONAL COMPLEXITY

There are non-solvable problems like the halting problem of TM (Sec. VIII.A). In fact, their number is uncountable. On the other hand, solvable problems can be classified according to their difficulty. There are easy problems (computationally *tractable*), like computing the determinant of any $n \times n$ matrix, and there are difficult problems (computationally *hard* or *untractable*), like computing the permanent of the same matrix.⁷⁶

The *complexity classes* have been devised to group solvable problems according to their degree of difficulty. Three aspects are addressed (Nielsen and Chuang, 2000): 1/ time or space resources required by its solution, 2/ the machine used in its solution (DTM, NDTM, PTM, or QTM), and 3/ the type of problem (decision, number of solutions, optimization, etc.).

A. Classical Complexity Classes

When the computation is done with DTMs or NDTMs, the relevant classes are the following (Papadimitriou,

⁷⁶The definition of the permanent is similar to the determinant. In fact the only difference is the missing sign of the permutations.

1994; Welsh, 1995; Yan, 2000; Salomaa 1989; Li and Vitányi, 1997).⁷⁷

i/ Class **P** (Polynomial), containing those problems that a DTM solves in *polynomial time*, i.e., the time taken for the DTM to find the solution increases at most polynomially with the length n (in bits) of the initial data.

Examples: 1/ arithmetic operations such as the addition and multiplication of integers, 2/ Euclid's algorithm, 3/ modular exponentiation, 4/ computation of determinants, 5/ sorting a list (SORT), and 6/ multiplication of points on elliptic curves by large integers.

ii/ Class **NP** (Nondeterministic Polynomial), containing those problems that a NDTM solves in polynomial time.⁷⁸

As there are not NDTMs in practice, it is convenient to know this other equivalent characterization of the **NP** class in which only DTMs are involved: a problem is **NP** if, given an arbitrary initial data x of binary length n , it admits any *succinct certificate* or *polynomial witness* y (i.e., of polynomial length in n), such that there exists a DTM which, with those data x, y , can solve the given problem in polynomial time in n .

Clearly, $\mathbf{P} \subseteq \mathbf{NP}$. A central conjecture in computation theory is $\mathbf{P} \not\subseteq \mathbf{NP}$.

Examples: 1/ the DISCRETE LOGARITHM problem (computation in \mathbb{Z}_N of the solution x to $a^x = b \bmod N$), 2/ the PRIMALITY problem (given N , is it prime?), 3/ COMPOSITENESS, complement to PRIMALITY (given N , is it composite?), 4/ the FACTORIZATION problem (find the decomposition of N into prime factors), 5/ the satisfiability problem SAT (check whether a given Boolean expression ϕ in normal conjunctive form $\phi = \bigwedge_1^n C_i$, $C_i := z_{i1} \vee z_{i2} \vee \dots \vee z_{ir_i}$, with $z_{ij} \in (x_{ij}, \neg x_{ij})$ Boolean variables or their negations, is satisfiable, that is, there exists a choice of variables that make ϕ true), and 6/ the traveling salesman problem TSD(D) (given n cities, their mutual distances $d_{ij} \geq 0$ and a cost or "travel budget", find whether there exists a cyclic permutation π such that $\sum_{i=1}^n d_{i,\pi(i)} \leq C$).

FACTORIZATION is **NP** since it is apparent that given N , and the succinct certificate consisting of its prime divisors, the decomposition of N into primes is trivial and of polynomial cost.

iii/ Class **PSPACE** (Polynomial Space) (**NSPACE**, Nondeterministic polynomial Space), containing those problems that some DTM (NDTM) solves in polynomial

⁷⁷Although the complexity classes **P**, **NP**, etc., that we shall consider here usually contain only decision problems (problems whose solution is either YES (1) or NO (0)), we shall implicitly enlarge them by including other computational problems, searching, etc., which are defined in a similar fashion to decision problems by means of the costs in time or space invested in its solution.

⁷⁸As there may be several computational pathways leading to the solution, the one of shortest duration marks the cost (Salomaa, 1989).

space, i.e., using a number of cells that grows at most polynomially with the length (in bits) of the initial data.

It is known that $\mathbf{NP} \subseteq \mathbf{PSPACE} = \mathbf{NSPACE}$.

Examples: 1/ In the two-players game GEOGRAPHY, player A chooses the name of a city, say MADRID, and B has to name another city, like DUBLIN, starting with the last letter D of the previous city; then the turn is on A for naming another city starting with N, like NEWYORK, B says next KYOTO, and so on and so forth. The cities' names must not be repeated. The loser is the player who cannot name another city because there are not more names left. The GEOGRAPHY problem is: given an arbitrary set of cities (strings, all different, of alphabet symbols), and A 's initial choice of one of them, can A win?. It can be shown that GEOGRAPHY is \mathbf{PSPACE} -complete.⁷⁹ 2/ Also the game GO suggests a GO problem on $n \times n$ boards and the associated question of whether there exists some winning strategy for the starting player. This GO Problem is likewise \mathbf{PSPACE} -complete.

iv/ Class \mathbf{EXP} (Exponential) (\mathbf{NEXP} , (Nondeterministic Exponential)), containing those problems that some DTM (NDTM) solves in exponential time, i.e., a time that grows at most exponentially with the length (in bits) of the initial data.

Examples: Consider the problems related to the games GO, CHECKERS and CHESS on $n \times n$ fields: are always there winning strategies for the first player? Since the number of movements to analyse grows exponentially with the board size, such problems are in \mathbf{EXP} . Furthermore, it is believed that they are not in class \mathbf{NP} .

The following inclusions among the previous classes hold:

$$\mathbf{P} \subseteq \mathbf{NP} \subseteq \mathbf{PSPACE} \subseteq \mathbf{EXP} \subseteq \mathbf{NEXP}.$$

Moreover, it is also known that $\mathbf{P} \subsetneq \mathbf{EXP}$. Thus, at least one of the three first inclusions in the long previous chain must be proper. But it is ignored which one.

The classification does not end here. There are even more “monstrous” problems, as far as complexity is concerned. For instance, pertaining to the Presburger arithmetic there exists a problem doubly exponential at least (time complexity $O(2^{2^n})$ in the size n of the initial data).

Let us now assume that our computers are PTMs. The corresponding classes are called *random*, and some of them stand out:

i/ Class \mathbf{RP} (Randomized Polynomial), consisting of those decision problems that a PTM T , always working in polynomial time (for every initial data), decides with error $\leq \frac{1}{2}$. These problems are called polynomial Monte Carlo. In other words, if L denotes the set of input data

having answer YES, i.e., 1, then

$$\begin{aligned} x \in L &\implies \text{prob}(T(x) = 1) \geq \frac{1}{2}, \\ x \notin L &\implies \text{prob}(T(x) = 1) = 0. \end{aligned}$$

This means that all computational pathways that a PTM T can take from a data $x \notin L$ end up with rejection ($T(x) = 0$, i.e., NO), while if $x \in L$, then at least a fraction $\frac{1}{2}$ of the possible paths end up with acceptance ($T(x) = 1$). Therefore, there cannot be false positives, and at most a fraction $\frac{1}{2}$ of false negatives can happen (cases in which $x \in L$ and however the followed path ends with rejection). Repeating the computation with the same $x \in L$ a number of times $n \gtrsim \lceil \log_2 \delta^{-1} \rceil$, where $0 < \delta < 1$, we will be able to get that the probability of n consecutive false negatives be $\leq \delta$ and thus as small as desired by appropriately choosing δ , or equivalently, that the probability to obtain in that series of n trials some acceptance of x be $\geq (1 - \delta)$ and thus as close to 1 as we wish. In cases of real “bad luck” it might happen that very long series would not contain any acceptance of x ; that is why it is often said that such T decides the problem in average case polynomial time.

ii/ Class $\mathbf{ZPP} := \mathbf{RP} \cap \mathbf{coRP}$ (Zero-error Probabilistic Polynomial), where the class \mathbf{coRP} is the complement of \mathbf{RP} , that is, it contains those decision problems that answer (YES, NO) to an input iff there exists a problem in \mathbf{RP} which answers (NO, YES) to the same input.

The class \mathbf{ZPP} thus contains those decision problems for which there exist two PTM $T_{\mathbf{RP}}$ and $T_{\mathbf{coRP}}$, always working in polynomial time and satisfying

$$\begin{aligned} x \in L &\implies \text{prob}(T_{\mathbf{RP}}(x) = 1) \geq \frac{1}{2}, \text{prob}(T_{\mathbf{coRP}}(x) = 1) = 0, \\ x \notin L &\implies \text{prob}(T_{\mathbf{RP}}(x) = 1) = 0, \text{prob}(T_{\mathbf{coRP}}(x) = 1) \geq \frac{1}{2}. \end{aligned}$$

These problems are called polynomial Las Vegas: they are Monte Carlo, and so are their complements. In other words, they have two Monte Carlo algorithms, one without false positives, and another one without false negatives. Most likely any input data will be decidable with certainty: it is enough that the algorithm without false positives says YES, or the one without false negatives says NO. In case of real bad luck, we shall have to repeat both until one of them yields a conclusive answer.

Example: PRIMALITY is in \mathbf{ZPP} . The Miller-Selfridge-Rabin algorithm (pseudo-primality strong test, 1974) is of coMonteCarlo type, that is, PRIMALITY is in \mathbf{coRP} (in fact, the probability of false positives, i.e., that one probable prime be composite, is $\leq 1/4$). That PRIMALITY is also in \mathbf{RP} is a harder issue, and was proved by Adleman and Huang (1987), with the theory of Abelian varieties (generalization of elliptic curves to higher dimensions).⁸⁰

⁷⁹Given a complexity class \mathbf{X} , a decision problem $P \in \mathbf{X}$ is called \mathbf{X} -complete when any $Q \in \mathbf{X}$ is polynomially reducible to P , i.e., \exists a polynomial-time map $f : x \mapsto f(x)$ from the inputs of Q to the inputs of P such that $Q(x) = 0, 1$ iff $P(f(x)) = 0, 1$.

⁸⁰Given an integer N , there exists a deterministic primality-

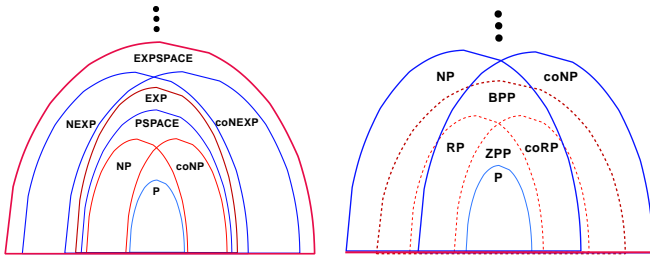


FIG. 57: Different classical complexity classes. On the right, we provisionally accept that **BPP** class is not a subset of **NP**.

iii/ Class **BPP** (Bounded-error Probabilistic Polynomial). It contains those decision problems for which there exists a PTM T always working in polynomial time and satisfying

$$\begin{aligned} x \in L &\implies \text{prob}(T(x) = 1) \geq \frac{3}{4}, \\ x \notin L &\implies \text{prob}(T(x) = 1) \leq \frac{1}{4}. \end{aligned}$$

BPP problems are perhaps those representing best the notion of realistic computations. They are accepted or rejected by a PTM with the possibility to err. But the error probability is $\leq \frac{1}{4}$ both on the acceptance as well as on the rejection. Repetition of the algorithm with the same input allows to amplify the probability of success, and, using the majority rule, to decide within polynomial time (average case time, except in bad luck instances) and with an error as small as required. It is not known whether $\mathbf{BPP} \subseteq \mathbf{NP}$, although it is believed that $\mathbf{NP} \not\subseteq \mathbf{BPP}$. It is clear that $\mathbf{RP} \subseteq \mathbf{BPP}$, and likewise $\mathbf{BPP} = \mathbf{coBPP}$. Generically:

$$\begin{aligned} \mathbf{P} \subseteq \mathbf{ZPP} \subseteq \mathbf{RP} \subseteq (\mathbf{BPP}, \mathbf{NP}) \subseteq \\ \subseteq \mathbf{PSPACE} \subseteq \mathbf{EXP} \subseteq \mathbf{NEXP}. \end{aligned}$$

Fig. 57 shows the inclusions among the classical complexity classes (Papadimitriou, 1995).

B. Quantum Complexity Classes

When the computers employed in the computations are QTM, the associated complexity classes are called quantum. We shall quote some of the most relevant:

i/ Class **QP** (Quantum Polynomial), containing those (decision) problems solvable in polynomial time with a QTM.

ii/ Class **BQP** (Bounded-error Quantum Polynomial). It contains those problems solvable with error $\leq 1/4$ in polynomial time with a QTM.

iii/ Class **ZQP** (Zero-error probability Quantum Polynomial). Set of problems solvable with zero error probability in expected polynomial time with a QTM.

The following relations with the classical complexity classes hold:

$$\mathbf{P} \subsetneq \mathbf{QP}, \quad \mathbf{BPP} \subseteq \mathbf{BQP} \subseteq \mathbf{PSPACE}.$$

The proper inclusion of **P** in **QP**, shown by Berthiaume and Brassard (1992), is very remarkable. It means that quantum computers can solve efficiently more problems than their classical kin. It amounts to the first clear victory in the strict separation of classical and quantum complexities.

The second chain of inclusions is due to Bernstein and Vazirani (1993). It remains open the crucial question of whether $\mathbf{BPP} \subsetneq \mathbf{BQP}$ or not. That is, are there quantum “tractable” problems which are classically hard? Simon’s algorithm (Subsec. X.B) is a first positive indication in the presence of a quantum oracle. Another fact supporting this point comes from Shor’s algorithm (Subsec. X.D), showing that FACTORIZATION and DISCRETE LOGARITHM are in **BQP**, whereas the current state of the art does not allow us to assert that they are in **BPP**. The inclusion of **BQP** in **PSPACE** implies that it is possible to classically simulate, and with as good approximation as desired, quantum problems with reasonable memory resources, although the simulation would be exponentially slow in time. That is why there are not solvable problems with QTMs escaping the domain of DTMs. Stated in a different way, quantum computation does not contradict the Church-Turing hypothesis (Subsec. VIII.A). Only invoking efficiency might classical TMs yield to QTMs.

Even though we do not know whether **BPP** is a proper subset of **BQP**, we do know classical particular cases of algorithms (not complexity classes as a whole) that can be speeded-up quantumly with respect to their classical running. Simon’s algorithm shows an exponential gain $O(2^n) \rightarrow O(n)$ (Subsec. X.B), and Grover’s shows a quadratic improvement $O(N) \rightarrow O(N^{1/2})$ (Subsec. X.C). But is not always possible to speed-up the algorithm substantially. There are oracle problems which do not admit an essential quantum speed-up; at the most it is possible to go from N classical queries down to $N/2$ quantum queries. An example is the PARITY problem (to find the parity of the number of non-zero bits of a string in $\{0, 1\}^n$, (Farhi et al., 1998)).

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testing algorithm, due to Adleman-Pomerance-Rumely-Cohen-Lenstra (1980-81), with complexity $O((\log_2 N)^c \log_2 \log_2 \log_2 N)$, where c is a constant. A current typical computer takes about 30 s for N with 100 decimal digits, about 8 min if N has 200 digits, and a reasonable time for 1000 digits.

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